Introduction to Machine Learning: Linear Learners

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Modeling the Frog's Perceptual System

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- [Lettvin et al. 1959] show that the frog's perceptual system constructs reality by four separate operations:
  - contrast detection: presence of sharp boundary?
  - convexity detection: how curved and how big is object?
  - movement detection: is object moving?
  - dimming speed: how fast does object obstruct light?
- The frog's goal: Capture any object of the size of an insect or worm providing it moves like one.

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  - movement detection: is object moving?
  - dimming speed: how fast does object obstruct light?
- The frog's goal: Capture any object of the size of an insect or worm providing it moves like one.
- Can we build a model of this perceptual system and learn to capture the right objects?

Learning from Data

- Assume training data of edible (+) and inedible (-) objects

convex	speed	label	convex	speed	label
small	small	-	small	large	+
small	medium	-	medium	large	+
small	medium	-	medium	large	+
medium	small	-	large	small	+
large	small	-	large	large	+
small	small	-	large	medium	+
small	large	-			
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  - p(+) = , p(-) =
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    $p(\text{speed} = \text{small}|+) = 1/6$, $p(\text{speed} = \text{med}|+) = 1/6$, $p(\text{speed} = \text{large}|+) = 4/6$
- Predict unseen $p(\text{label} = ?, \text{convex} = \text{med}, \text{speed} = \text{med})$
  - $p(-) \cdot p(\text{convex} = \text{med}|-) \cdot p(\text{speed} = \text{med}|-) =$
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  - $p(+) \cdot p(\text{convex} = \text{med}|+) \cdot p(\text{speed} = \text{med}|+) = 6/14 \cdot 2/6 \cdot 1/6 = 0.024$

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    p(speed = small|+) = 1/6, p(speed = med|+) = 1/6, p(speed = large|+) = 4/6
- Predict unseen p(label = ?, convex = med, speed = med)
  - p(-) · p(convex = med|-) · p(speed = med|-) = 8/14 · 1/8 · 3/8 = 0.027
  - p(+) · p(convex = med|+) · p(speed = med|+) = 6/14 · 2/6 · 1/6 = 0.024
  - Inedible: p(convex = med, speed = med, label = -) > p(convex = med, speed = med, label = +)!

Machine Learning is a Frog's World

- Machine learning problems can be seen as problems of function estimation where
  - our models are based on a combined feature representation of inputs and outputs
    - *similar to the frog whose world is constructed by four-dimensional feature vector based on detection operations*

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  - learning of parameter weights is done by optimizing fit of model to training data
    - *frog uses binary classification into edible/inedible objects as supervision signals for learning*
  - The model used in the frog's perception example is called *Naive Bayes*: It measures compatibility of inputs to outputs by a linear model and optimizes parameters by convex optimization

Lecture Outline

- Preliminaries
  - Data: input/output
  - Feature representations
  - Linear models
- Convex optimization for linear models
  - Naive Bayes
  - Generative versus discriminative
  - Logistic Regression
  - Perceptron
  - Large-Margin Learners (SVMs)
- Regularization
- Online learning
- Non-linear models

Inputs and Outputs

- Input: $\boldsymbol{x} \in \mathcal{X}$
  - e.g., document or sentence with some words $\boldsymbol{x} = w_1 \ldots w_n$
- Output: $\boldsymbol{y} \in \mathcal{Y}$
  - e.g., document class, translation, parse tree

- Input/Output pair: $(\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{X} \times \mathcal{Y}$
  - e.g., a document $\boldsymbol{x}$ and its class label $\boldsymbol{y}$,
  - a source sentence $\boldsymbol{x}$ and its translation $\boldsymbol{y}$,
  - a sentence $\boldsymbol{x}$ and its parse tree $\boldsymbol{y}$

Feature Representations

- Most NLP problems can be cast as multiclass classification where we assume a high-dimensional joint feature map on input-output pairs $(\boldsymbol{x}, \boldsymbol{y})$
  - $\boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}) : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}^m$

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  - $\boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}) : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^m$
- Common ranges:
  - categorical (e.g., counts): $\phi_i \in \{1, \ldots, F_i\}$, $F_i \in \mathbb{N}^+$
  - binary (e.g., binning): $\boldsymbol{\phi} \in \{0, 1\}^m$
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  - continuous (e.g., word embeddings): $\boldsymbol{\phi} \in \mathbb{R}^m$
- For any vector $\mathbf{v} \in \mathbb{R}^m$, let $\mathbf{v}_j$ be the j^{th} value

Examples

- $\boldsymbol{x}$ is a document and $\boldsymbol{y}$ is a label

$$\phi_j(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \text{ contains the word ``interest''} \\ & \text{and } \boldsymbol{y} = \text{``financial''} \\ 0 & \text{otherwise} \end{cases}$$

We expect this feature to have a positive weight, “interest” is a positive indicator for the label “financial”

Examples

$\phi_j(\boldsymbol{x}, \boldsymbol{y}) =$ % of words in $\boldsymbol{x}$ containing punctuation and $\boldsymbol{y} =$ "scientific"

Punctuation symbols - positive indicator or negative indicator for scientific articles?

Examples

- $\boldsymbol{x}$ is a word and $\boldsymbol{y}$ is a part-of-speech tag

$$\phi_j(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} 1 & \text{if } \boldsymbol{x} = \text{ ``bank'' and } \boldsymbol{y} = \text{ Verb} \\ 0 & \text{otherwise} \end{cases}$$

What weight would it get?

Examples

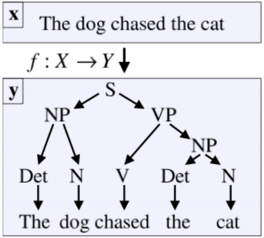
- $\boldsymbol{x}$ is a source sentence and $\boldsymbol{y}$ is translation

$$\phi_j(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} 1 & \text{if "y a-t-il" present in } \boldsymbol{x} \\ & \quad \text{and "are there" present in } \boldsymbol{y} \\ 0 & \text{otherwise} \end{cases}$$

$$\phi_k(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} 1 & \text{if "y a-t-il" present in } \boldsymbol{x} \\ & \quad \text{and "are there any" present in } \boldsymbol{y} \\ 0 & \text{otherwise} \end{cases}$$

Which phrase indicator should be preferred?

Examples



$$\Psi(\mathbf{x},\mathbf{y}) = \begin{pmatrix} 1 \\ 0 \\ 2 \\ 1 \\ \vdots \\ 0 \\ 2 \\ 1 \\ 1 \\ 1 \end{pmatrix} \begin{array}{c} S \rightarrow NP\ VP \\ S \rightarrow NP \\ NP \rightarrow Det\ N \\ VP \rightarrow V\ NP \\ \\ Det \rightarrow dog \\ Det \rightarrow the \\ N \rightarrow dog \\ V \rightarrow chased \\ N \rightarrow cat \end{array}$$

Note: Label $\boldsymbol{y}$ includes sentence $\boldsymbol{x}$

Linear Models

- **Linear model**: Defines a discriminant function that is based on linear combination of features and weights

$$
\begin{aligned}
f(\boldsymbol{x}; \boldsymbol{\omega}) &= \underset{\boldsymbol{y} \in \mathcal{Y}}{\arg\max}\ \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}) \\
&= \underset{\boldsymbol{y} \in \mathcal{Y}}{\arg\max}\ \sum_{j=0}^{m} \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}, \boldsymbol{y})
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\end{aligned}
$$

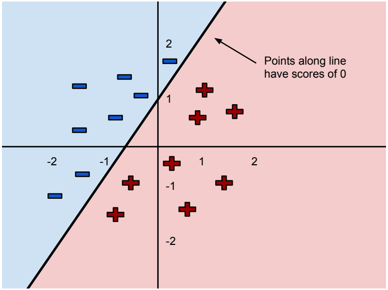
- Let $\boldsymbol{\omega} \in \mathbb{R}^m$ be a high dimensional weight vector
- Assume that $\boldsymbol{\omega}$ is known
  - **Multiclass Classification**: $\mathcal{Y} = \{0, 1, \ldots, N\}$

$$
\boldsymbol{y} = \arg\max_{\boldsymbol{y}'\in\mathcal{Y}} \ \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y}')
$$

  - **Binary Classification** just a special case of multiclass

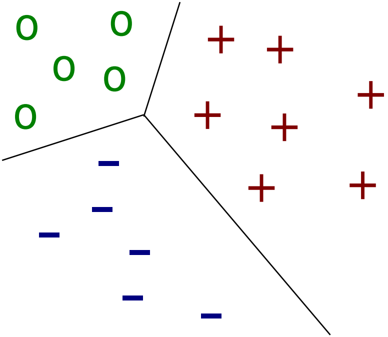
Linear Models for Binary Classification

- ω defines a linear decision boundary that divides space of instances in two classes
  - 2 dimensions: line
  - 3 dimensions: plane
  - n dimensions: hyperplane of $n-1$ dimensions



Multiclass Linear Model

Defines regions of space. Visualization difficult.



- $+$ are all points $(\boldsymbol{x}, \boldsymbol{y})$ where $+ = \arg\max_{\boldsymbol{y}}\ \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y})$

Convex Optimization for Supervised Learning

How to learn weight vector $\boldsymbol{\omega}$ in order to make decisions?

- Input:
  - i.i.d. (independent and identically distributed) training examples $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$
  - feature representation ϕ

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  - feature representation ϕ
- Output: $\boldsymbol{\omega}$ that maximizes an objective function on the training set
  - $\boldsymbol{\omega} = \arg\max \mathcal{L}(\mathcal{T}; \boldsymbol{\omega})$
  - Equivalently minimize: $\boldsymbol{\omega} = \arg\min -\mathcal{L}(\mathcal{T}; \boldsymbol{\omega})$

Objective Functions

- Ideally we can decompose $\mathcal{L}$ by training pairs $(\boldsymbol{x}, \boldsymbol{y})$
  - $\mathcal{L}(\mathcal{T}; \boldsymbol{\omega}) \propto \sum_{(\boldsymbol{x},\boldsymbol{y})\in\mathcal{T}} \mathit{loss}((\boldsymbol{x}, \boldsymbol{y}); \boldsymbol{\omega})$
  - *loss* is a function that measures some value correlated with errors of parameters $\boldsymbol{\omega}$ on instance $(\boldsymbol{x}, \boldsymbol{y})$

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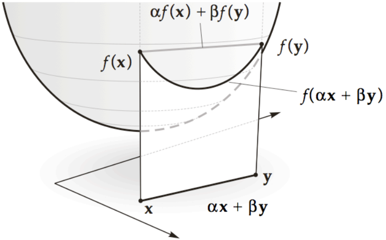
  - *loss* is a function that measures some value correlated with errors of parameters $\boldsymbol{\omega}$ on instance $(\boldsymbol{x}, \boldsymbol{y})$
- Example:
  - $\boldsymbol{y} \in \{1, -1\}$, $f(\boldsymbol{x}; \boldsymbol{\omega})$ is the prediction we make for $\boldsymbol{x}$ using $\boldsymbol{\omega}$
  - 0-1 loss function: $loss((\boldsymbol{x}, \boldsymbol{y}); \boldsymbol{\omega}) = \begin{cases} 0 & \text{if } f(\boldsymbol{x}; \boldsymbol{\omega}) = \boldsymbol{y}, \\ 1 & \text{else} \end{cases}$

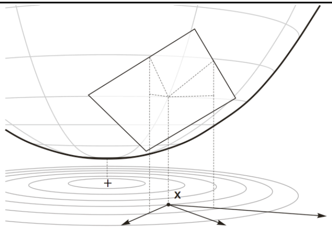
Convexity



- A function is convex if its graph lies on or below the line segment connecting any two points on the graph

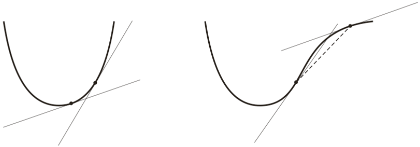
$$f(\alpha \boldsymbol{x} + \beta \boldsymbol{y}) \leq \alpha f(\boldsymbol{x}) + \beta f(\boldsymbol{y}) \text{ for all } \alpha, \beta \geq 0, \ \alpha + \beta = 1 \quad (1)$$

Gradient



- Gradient of function f is vector of partial derivatives.
  $\nabla f(x) = \left(\frac{\partial}{\partial x_1} f(x), \frac{\partial}{\partial x_2} f(x), ..., \frac{\partial}{\partial x_n} f(x) \right)$
- Rate of increase of f at point x in each of the axis-parallel directions.

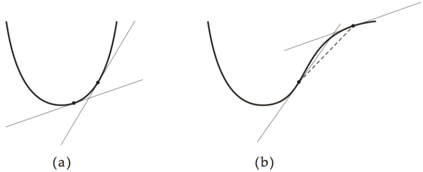
Convex Optimization



(a) (b)

- Optimization problem is defined as problem of finding a point that minimizes our objective function (maximization is minimization of $-f(x)$)

Convex Optimization



- Optimization problem is defined as problem of finding a point that minimizes our objective function (maximization is minimization of $-f(x)$)
- In order to find minimum, follow opposite direction of gradient
- For convex (or linear) functions, global minimum at point where $\nabla f(x) = 0$

Naive Bayes

Naive Bayes

- Probabilistic decision model:

$$\arg\max_{\boldsymbol{y}} P(\boldsymbol{y}|\boldsymbol{x}) \propto \arg\max_{\boldsymbol{y}} P(\boldsymbol{y})P(\boldsymbol{x}|\boldsymbol{y})$$

  - Uses Bayes Rule:

$$P(\boldsymbol{y}|\boldsymbol{x}) = \frac{P(\boldsymbol{y})P(\boldsymbol{x}|\boldsymbol{y})}{P(\boldsymbol{x})} \text{ for fixed } \boldsymbol{x}$$

- Generative model since $P(\boldsymbol{y})P(\boldsymbol{x}|\boldsymbol{y}) = P(\boldsymbol{x}, \boldsymbol{y})$ is a joint probability
  - Because we model a distribution that can randomly generate outputs *and* inputs, not just outputs

Naivety of Naive Bayes

- We need to decide on the structure of $P(\boldsymbol{x}, \boldsymbol{y})$
- $P(\boldsymbol{x}|\boldsymbol{y}) = P(\phi(\boldsymbol{x})|\boldsymbol{y}) = P(\phi_1(\boldsymbol{x}), \ldots, \phi_m(\boldsymbol{x})|\boldsymbol{y})$

Naive Bayes Assumption

(conditional independence)

$$P(\phi_1(\boldsymbol{x}), \ldots, \phi_m(\boldsymbol{x})|\boldsymbol{y}) = \prod_i P(\phi_i(\boldsymbol{x})|\boldsymbol{y})$$

- $P(\boldsymbol{x}, \boldsymbol{y}) = P(\boldsymbol{y}) \prod_{i=1}^m P(\phi_i(\boldsymbol{x})|\boldsymbol{y})$

Naive Bayes – Learning

- Input: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$
- Let $\phi_i(\boldsymbol{x}) \in \{1, \ldots, F_i\}$
- Parameters $\mathcal{P} = \{P(\boldsymbol{y}), P(\phi_i(\boldsymbol{x})|\boldsymbol{y})\}$

Maximum Likelihood Estimation

- What's left? Defining an objective $\mathcal{L}(\mathcal{T})$
- $\mathcal{P}$ plays the role of $\boldsymbol{\omega}$
- What objective to use?
- Objective: Maximum Likelihood Estimation (MLE)

$$\mathcal{L}(\mathcal{T}) = \prod_{t=1}^{|\mathcal{T}|} P(\boldsymbol{x}_t, \boldsymbol{y}_t) = \prod_{t=1}^{|\mathcal{T}|} \left(P(\boldsymbol{y}_t) \prod_{i=1}^{m} P(\phi_i(\boldsymbol{x}_t)|\boldsymbol{y}_t) \right)$$

Naive Bayes – Learning

MLE has closed form solution

$$\mathcal{P} = \arg\max_{\mathcal{P}} \prod_{t=1}^{|\mathcal{T}|} \left(P(\boldsymbol{y}_t) \prod_{i=1}^{m} P(\phi_i(\boldsymbol{x}_t)|\boldsymbol{y}_t) \right)$$

$$P(\boldsymbol{y}) = \frac{\sum_{t=1}^{|\mathcal{T}|} [\![\boldsymbol{y}_t = \boldsymbol{y}]\!]}{|\mathcal{T}|}$$

$$P(\phi_i(\boldsymbol{x})|\boldsymbol{y}) = \frac{\sum_{t=1}^{|\mathcal{T}|} [\![\phi_i(\boldsymbol{x}_t) = \phi_i(\boldsymbol{x}) \text{ and } \boldsymbol{y}_t = \boldsymbol{y}]\!]}{\sum_{t=1}^{|\mathcal{T}|} [\![\boldsymbol{y}_t = \boldsymbol{y}]\!]}$$

$$\text{where } [\![p]\!] = \begin{cases} 1 & \text{if } p \text{ is true,} \\ 0 & \text{otherwise.} \end{cases}$$

Thus, these are just normalized counts over events in $\mathcal{T}$

Deriving MLE

$$\mathcal{P} = \arg\max_{\mathcal{P}} \prod_{t=1}^{|\mathcal{T}|} \left(P(\boldsymbol{y}_t) \prod_{i=1}^{m} P(\phi_i(\boldsymbol{x}_t)|\boldsymbol{y}_t) \right)$$

Deriving MLE

$$
\begin{aligned}
\mathcal{P} &= \arg\max_{\mathcal{P}} \prod_{t=1}^{|\mathcal{T}|} \left(P(\boldsymbol{y}_t) \prod_{i=1}^{m} P(\phi_i(\boldsymbol{x}_t)|\boldsymbol{y}_t) \right) \\
&= \arg\max_{\mathcal{P}} \sum_{t=1}^{|\mathcal{T}|} \left(\log P(\boldsymbol{y}_t) + \sum_{i=1}^{m} \log P(\phi_i(\boldsymbol{x}_t)|\boldsymbol{y}_t) \right) \\
&= \arg\max_{P(\boldsymbol{y})} \sum_{t=1}^{|\mathcal{T}|} \log P(\boldsymbol{y}_t) + \arg\max_{P(\phi_i(\boldsymbol{x})|\boldsymbol{y})} \sum_{t=1}^{|\mathcal{T}|} \sum_{i=1}^{m} \log P(\phi_i(\boldsymbol{x}_t)|\boldsymbol{y}_t)
\end{aligned}
$$

such that $\sum_{\boldsymbol{y}} P(\boldsymbol{y}) = 1$, $\sum_{j=1}^{F_i} P(\phi_i(\boldsymbol{x}) = j|\boldsymbol{y}) = 1$, $P(\cdot) \geq 0$

Deriving MLE

$$\mathcal{P} = \operatorname*{arg\,max}_{P(\boldsymbol{y})} \sum_{t=1}^{|\mathcal{T}|} \log P(\boldsymbol{y}_t) + \operatorname*{arg\,max}_{P(\phi_i(\boldsymbol{x})|\boldsymbol{y})} \sum_{t=1}^{|\mathcal{T}|} \sum_{i=1}^{m} \log P(\phi_i(\boldsymbol{x}_t)|\boldsymbol{y}_t)$$

Deriving MLE

$$\mathcal{P} = \arg\max_{P(\boldsymbol{y})} \sum_{t=1}^{|\mathcal{T}|} \log P(\boldsymbol{y}_t) + \arg\max_{P(\phi_i(\boldsymbol{x})|\boldsymbol{y})} \sum_{t=1}^{|\mathcal{T}|} \sum_{i=1}^{m} \log P(\phi_i(\boldsymbol{x}_t)|\boldsymbol{y}_t)$$

Both optimizations are of the form

$$\arg\max_P \sum_v \text{count}(v) \log P(v), \text{ s.t. } \sum_v P(v) = 1,\ P(v) \geq 0$$

where v is event in $\mathcal{T}$, either $(\boldsymbol{y}_t = \boldsymbol{y})$ or $(\phi_i(\boldsymbol{x}_t) = \phi_i(\boldsymbol{x}), \boldsymbol{y}_t = \boldsymbol{y})$

Deriving MLE

$$\arg\max_P \sum_v \mathsf{count}(v) \log P(v)$$
$$\text{s.t., } \sum_v P(v) = 1,\ P(v) \geq 0$$

Introduce Lagrangian multiplier λ, optimization becomes

$$\arg\max_{P,\lambda}\ \sum_v \mathsf{count}(v) \log P(v) - \lambda \left(\sum_v P(v) - 1\right)$$

Deriving MLE

$$\arg\max_P \sum_v \text{count}(v) \log P(v)$$
$$\text{s.t.}, \sum_v P(v) = 1,\ P(v) \geq 0$$

Introduce Lagrangian multiplier λ, optimization becomes

$$\arg\max_{P,\lambda}\ \sum_v \text{count}(v) \log P(v) - \lambda \left(\sum_v P(v) - 1\right)$$

- Derivative w.r.t $P(v)$ is $\frac{\text{count(v)}}{P(v)} - \lambda$
- Setting this to zero $P(v) = \frac{\text{count(v)}}{\lambda}$
- Use $\sum_v P(v) = 1$, $P(v) \geq 0$, then $P(v) = \frac{\text{count(v)}}{\sum_{v'} \text{count}(v')}$

Deriving MLE

Reinstantiate events v in $\mathcal{T}$:

$$P(\boldsymbol{y}) = \frac{\sum_{t=1}^{|\mathcal{T}|} [\![\boldsymbol{y}_t = \boldsymbol{y}]\!]}{|\mathcal{T}|}$$

$$P(\phi_i(\boldsymbol{x})|\boldsymbol{y}) = \frac{\sum_{t=1}^{|\mathcal{T}|} [\![\phi_i(\boldsymbol{x}_t) = \phi_i(\boldsymbol{x}) \text{ and } \boldsymbol{y}_t = \boldsymbol{y}]\!]}{\sum_{t=1}^{|\mathcal{T}|} [\![\boldsymbol{y}_t = \boldsymbol{y}]\!]}$$

Naive Bayes is a linear model

- Let $\boldsymbol{\omega}_{\boldsymbol{y}} = \log P(\boldsymbol{y})$, $\forall \boldsymbol{y} \in \mathcal{Y}$
- Let $\boldsymbol{\omega}_{\phi_i(\boldsymbol{x}),\boldsymbol{y}} = \log P(\phi_i(\boldsymbol{x})|\boldsymbol{y})$, $\forall \boldsymbol{y} \in \mathcal{Y}, \phi_i(\boldsymbol{x}) \in \{1, \ldots, F_i\}$

Naive Bayes is a linear model

- Let $\omega_{\boldsymbol{y}} = \log P(\boldsymbol{y}), \forall \boldsymbol{y} \in \mathcal{Y}$
- Let $\omega_{\phi_i(\boldsymbol{x}),\boldsymbol{y}} = \log P(\phi_i(\boldsymbol{x})|\boldsymbol{y}), \forall \boldsymbol{y} \in \mathcal{Y}, \phi_i(\boldsymbol{x}) \in \{1, \ldots, F_i\}$

$$
\begin{aligned}
\arg\max_{\boldsymbol{y}} \; P(\boldsymbol{y}|\phi(\boldsymbol{x})) \quad & \propto \quad \arg\max_{\boldsymbol{y}} \; P(\phi(\boldsymbol{x}), \boldsymbol{y}) = \arg\max_{\boldsymbol{y}} \; P(\boldsymbol{y}) \prod_{i=1}^{m} P(\phi_i(\boldsymbol{x})|\boldsymbol{y}) \\
& = \quad \arg\max_{\boldsymbol{y}} \; \log P(\boldsymbol{y}) + \sum_{i=1}^{m} \log P(\phi_i(\boldsymbol{x})|\boldsymbol{y}) \\
& = \quad \arg\max_{\boldsymbol{y}} \; \omega_{\boldsymbol{y}} + \sum_{i=1}^{m} \omega_{\phi_i(\boldsymbol{x}),\boldsymbol{y}} \\
& = \quad \arg\max_{\boldsymbol{y}} \; \sum_{\boldsymbol{y}'} \omega_{\boldsymbol{y}} \psi_{\boldsymbol{y}'}(\boldsymbol{y}) + \sum_{i=1}^{m} \sum_{j=1}^{F_i} \omega_{\phi_i(\boldsymbol{x}),\boldsymbol{y}} \psi_{i,j}(\boldsymbol{x})
\end{aligned}
$$

where $\psi_{i,j}(\boldsymbol{x}) = [\![\phi_i(\boldsymbol{x}) = j]\!]$, $\psi_{\boldsymbol{y}'}(\boldsymbol{y}) = [\![\boldsymbol{y} = \boldsymbol{y}']\!]$

Discriminative versus Generative Models

- Generative models attempt to model inputs and outputs
  - e.g., Naive Bayes = MLE of joint distribution $P(\boldsymbol{x}, \boldsymbol{y})$
  - Statistical model must explain generation of input
- Occam's Razor: "Among competing hypotheses, the one with the fewest assumptions should be selected"
- Discriminative models
  - Use $\mathcal{L}$ that directly optimizes $P(\boldsymbol{y}|\boldsymbol{x})$ (or something related)
  - Logistic Regression – MLE of $P(\boldsymbol{y}|\boldsymbol{x})$
  - Perceptron and SVMs – minimize classification error
- Generative and discriminative models use $P(\boldsymbol{y}|\boldsymbol{x})$ for prediction
- Differ only on what distribution they use to set $\boldsymbol{\omega}$

Logistic Regression

Logistic Regression

Define a conditional probability:

$$P(\boldsymbol{y}|\boldsymbol{x}) = \frac{e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y})}}{Z_{\boldsymbol{x}}}, \qquad \text{where } Z_{\boldsymbol{x}} = \sum_{\boldsymbol{y}'\in\mathcal{Y}} e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y}')}$$

Note: still a linear model

$$\begin{aligned}
\arg\max_{\boldsymbol{y}} \; P(\boldsymbol{y}|\boldsymbol{x}) &= \arg\max_{\boldsymbol{y}} \; \frac{e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y})}}{Z_{\boldsymbol{x}}} \\
&= \arg\max_{\boldsymbol{y}} \; e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y})} \\
&= \arg\max_{\boldsymbol{y}} \; \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y})
\end{aligned}$$

Logistic Regression

$$P(\boldsymbol{y}|\boldsymbol{x}) = \frac{e^{\boldsymbol{\omega}\cdot\phi(\boldsymbol{x},\boldsymbol{y})}}{Z_{\boldsymbol{x}}}$$

- Q: How do we learn weights $\boldsymbol{\omega}$
- A: Set weights to maximize log-likelihood of training data:

$$\begin{aligned}
\boldsymbol{\omega} &= \arg\max_{\boldsymbol{\omega}} \mathcal{L}(\mathcal{T};\boldsymbol{\omega}) \\
&= \arg\max_{\boldsymbol{\omega}} \prod_{t=1}^{|\mathcal{T}|} P(\boldsymbol{y}_t|\boldsymbol{x}_t) = \arg\max_{\boldsymbol{\omega}} \sum_{t=1}^{|\mathcal{T}|} \log P(\boldsymbol{y}_t|\boldsymbol{x}_t)
\end{aligned}$$

- In a nutshell we set the weights $\boldsymbol{\omega}$ so that we assign as much probability to the correct label $\boldsymbol{y}$ for each $\boldsymbol{x}$ in the training set

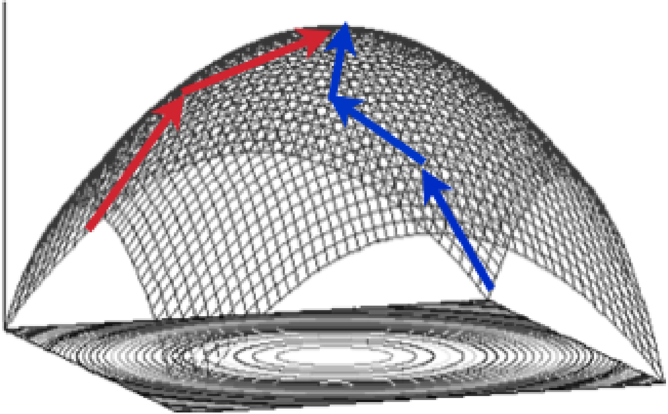
Logistic Regression

$$P(\boldsymbol{y}|\boldsymbol{x}) = \frac{e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y})}}{Z_{\boldsymbol{x}}}, \qquad \text{where } Z_{\boldsymbol{x}} = \sum_{\boldsymbol{y}'\in\mathcal{Y}} e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y}')}$$

$$\boldsymbol{\omega} = \arg\max_{\boldsymbol{\omega}} \sum_{t=1}^{|\mathcal{T}|} \log P(\boldsymbol{y}_t|\boldsymbol{x}_t) \ (*)$$

- The objective function (*) is concave
- Therefore there is a global maximum
- No closed form solution, but lots of numerical techniques
  - Gradient methods (gradient ascent, conjugate gradient, iterative scaling)
  - Newton methods (limited-memory quasi-newton)

Gradient Ascent



Gradient Ascent

- Let $\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = \sum_{t=1}^{|\mathcal{T}|} \log\left(e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)}/Z_{\boldsymbol{x}}\right)$
- Want to find $\arg\max_{\boldsymbol{\omega}} \mathcal{L}(\mathcal{T};\boldsymbol{\omega})$
  - Set $\boldsymbol{\omega}^0 = O^m$
  - Iterate until convergence

$$\boldsymbol{\omega}^i = \boldsymbol{\omega}^{i-1} + \alpha\nabla\mathcal{L}(\mathcal{T};\boldsymbol{\omega}^{i-1})$$

- $\alpha > 0$ is a step size / learning rate
- $\nabla\mathcal{L}(\mathcal{T};\boldsymbol{\omega})$ is gradient of $\mathcal{L}$ w.r.t. $\boldsymbol{\omega}$
  - A gradient is all partial derivatives over variables w_i
  - i.e., $\nabla\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = (\frac{\partial}{\partial\boldsymbol{\omega}_0}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}), \frac{\partial}{\partial\boldsymbol{\omega}_1}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}), \ldots, \frac{\partial}{\partial\boldsymbol{\omega}_m}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}))$

- Gradient ascent will always find $\boldsymbol{\omega}$ to maximize $\mathcal{L}$

Gradient Descent

- Let $\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = -\sum_{t=1}^{|\mathcal{T}|} \log\left(e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)}/Z_{\boldsymbol{x}}\right)$
- Want to find $\arg\min_{\boldsymbol{\omega}} \mathcal{L}(\mathcal{T};\boldsymbol{\omega})$
  - Set $\boldsymbol{\omega}^0 = O^m$
  - Iterate until convergence

$$\boldsymbol{\omega}^i = \boldsymbol{\omega}^{i-1} - \alpha\nabla\mathcal{L}(\mathcal{T};\boldsymbol{\omega}^{i-1})$$

- $\alpha > 0$ is step size / learning rate
- $\nabla\mathcal{L}(\mathcal{T};\boldsymbol{\omega})$ is gradient of $\mathcal{L}$ w.r.t. $\boldsymbol{\omega}$
  - A gradient is all partial derivatives over variables w_i
  - i.e., $\nabla\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = (\frac{\partial}{\partial\boldsymbol{\omega}_0}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}), \frac{\partial}{\partial\boldsymbol{\omega}_1}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}), \ldots, \frac{\partial}{\partial\boldsymbol{\omega}_m}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}))$
- Gradient descent will always find $\boldsymbol{\omega}$ to minimize $\mathcal{L}$

The partial derivatives

- Need to find all partial derivatives $\frac{\partial}{\partial \boldsymbol{\omega}_i}\mathcal{L}(\mathcal{T};\boldsymbol{\omega})$

$$
\begin{aligned}
\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) &= \sum_t \log P(\boldsymbol{y}_t|\boldsymbol{x}_t) \\
&= \sum_t \log \frac{e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)}}{\sum_{\boldsymbol{y}'\in\mathcal{Y}} e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}')}} \\
&= \sum_t \log \frac{e^{\sum_j \boldsymbol{\omega}_j\times\boldsymbol{\phi}_j(\boldsymbol{x}_t,\boldsymbol{y}_t)}}{Z_{\boldsymbol{x}_t}}
\end{aligned}
$$

Partial derivatives - some reminders

1. $\frac{\partial}{\partial x} \log F = \frac{1}{F} \frac{\partial}{\partial x} F$
   - We always assume log is the natural logarithm $\log_e$
2. $\frac{\partial}{\partial x} e^F = e^F \frac{\partial}{\partial x} F$
3. $\frac{\partial}{\partial x} \sum_t F_t = \sum_t \frac{\partial}{\partial x} F_t$
4. $\frac{\partial}{\partial x} \frac{F}{G} = \frac{G \frac{\partial}{\partial x} F - F \frac{\partial}{\partial x} G}{G^2}$

The partial derivatives

$$\frac{\partial}{\partial \omega_i} \mathcal{L}(\mathcal{T}; \omega) =$$

The partial derivatives (1)

$$
\begin{aligned}
\frac{\partial}{\partial \omega_i} \mathcal{L}(\mathcal{T};\boldsymbol{\omega}) &= \frac{\partial}{\partial \omega_i} \sum_t \log \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z_{\boldsymbol{x}_t}} \\
&= \sum_t \frac{\partial}{\partial \omega_i} \log \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z_{\boldsymbol{x}_t}} \\
&= \sum_t \left(\frac{Z_{\boldsymbol{x}_t}}{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}\right)\left(\frac{\partial}{\partial \omega_i} \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z_{\boldsymbol{x}_t}}\right)
\end{aligned}
$$

The partial derivatives

Now, $\frac{\partial}{\partial \boldsymbol{\omega}_i} \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z_{\boldsymbol{x}_t}} =$

The partial derivatives (2)

Now,

$$
\begin{aligned}
\frac{\partial}{\partial \boldsymbol{\omega}_i} \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z_{\boldsymbol{x}_t}} &= \frac{Z_{\boldsymbol{x}_t} \frac{\partial}{\partial \boldsymbol{\omega}_i} e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)} - e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)} \frac{\partial}{\partial \boldsymbol{\omega}_i} Z_{\boldsymbol{x}_t}}{Z^2_{\boldsymbol{x}_t}} \\
&= \frac{Z_{\boldsymbol{x}_t} e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}_t) - e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)} \frac{\partial}{\partial \boldsymbol{\omega}_i} Z_{\boldsymbol{x}_t}}{Z^2_{\boldsymbol{x}_t}} \\
&= \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z^2_{\boldsymbol{x}_t}} \left(Z_{\boldsymbol{x}_t} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}_t) - \frac{\partial}{\partial \boldsymbol{\omega}_i} Z_{\boldsymbol{x}_t}\right) \\
&= \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z^2_{\boldsymbol{x}_t}} \Big(Z_{\boldsymbol{x}_t} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}_t) \\
&\qquad - \sum_{\boldsymbol{y}' \in \mathcal{Y}} e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}')} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}')\Big)
\end{aligned}
$$

because

$$
\frac{\partial}{\partial \boldsymbol{\omega}_i} Z_{\boldsymbol{x}_t} = \frac{\partial}{\partial \boldsymbol{\omega}_i} \sum_{\boldsymbol{y}' \in \mathcal{Y}} e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}')} = \sum_{\boldsymbol{y}' \in \mathcal{Y}} e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}')} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}')
$$

The partial derivatives

The partial derivatives (3)

From (2),

$$\frac{\partial}{\partial \boldsymbol{\omega}_i} \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z_{\boldsymbol{x}_t}} = \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z^2_{\boldsymbol{x}_t}} (Z_{\boldsymbol{x}_t} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}_t) - \sum_{\boldsymbol{y}' \in \mathcal{Y}} e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}')} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}'))$$

Sub this in (1),

$$\begin{aligned}
\frac{\partial}{\partial \boldsymbol{\omega}_i} \mathcal{L}(\mathcal{T}; \boldsymbol{\omega}) &= \sum_t \left(\frac{Z_{\boldsymbol{x}_t}}{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}\right)\left(\frac{\partial}{\partial \boldsymbol{\omega}_i} \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}_t)}}{Z_{\boldsymbol{x}_t}}\right) \\
&= \sum_t \frac{1}{Z_{x_t}} (Z_{\boldsymbol{x}_t} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}_t) - \sum_{\boldsymbol{y}' \in \mathcal{Y}} e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}')} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}'))) \\
&= \sum_t \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}_t) - \sum_t \sum_{\boldsymbol{y}' \in \mathcal{Y}} \frac{e^{\sum_j \boldsymbol{\omega}_j \times \boldsymbol{\phi}_j(\boldsymbol{x}_t, \boldsymbol{y}')}}{Z_{x_t}} \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}') \\
&= \sum_t \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}_t) - \sum_t \sum_{\boldsymbol{y}' \in \mathcal{Y}} P(\boldsymbol{y}' | \boldsymbol{x}_t) \boldsymbol{\phi}_i(\boldsymbol{x}_t, \boldsymbol{y}')
\end{aligned}$$

FINALLY!!!

- After all that,

$$\frac{\partial}{\partial \omega_i}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) \quad = \quad \sum_t \phi_i(\boldsymbol{x}_t,\boldsymbol{y}_t) - \sum_t \sum_{\boldsymbol{y}'\in\mathcal{Y}} P(\boldsymbol{y}'|\boldsymbol{x}_t)\phi_i(\boldsymbol{x}_t,\boldsymbol{y}')$$

- And the gradient is:

$$\nabla\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = (\frac{\partial}{\partial \boldsymbol{\omega}_0}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}), \frac{\partial}{\partial \boldsymbol{\omega}_1}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}), \ldots, \frac{\partial}{\partial \boldsymbol{\omega}_m}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}))$$

- So we can now use gradient ascent to find ω!!

Logistic Regression Summary

- Define conditional probability

$$P(\boldsymbol{y}|\boldsymbol{x}) = \frac{e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{y})}}{Z_{\boldsymbol{x}}}$$

- Set weights to maximize log-likelihood of training data:

$$\boldsymbol{\omega} = \arg\max_{\boldsymbol{\omega}} \sum_t \log P(\boldsymbol{y}_t|\boldsymbol{x}_t)$$

- Can find the gradient and run gradient ascent (or any gradient-based optimization algorithm)

$$\frac{\partial}{\partial \omega_i}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = \sum_t \phi_i(\boldsymbol{x}_t,\boldsymbol{y}_t) - \sum_t \sum_{\boldsymbol{y}'\in\mathcal{Y}} P(\boldsymbol{y}'|\boldsymbol{x}_t)\phi_i(\boldsymbol{x}_t,\boldsymbol{y}')$$

Logistic Regression = Maximum Entropy

- Well-known equivalence
- Max Ent: maximize entropy subject to constraints on features: $P = \arg\max_P H(P)$ under constraints
  - Empirical feature counts must equal expected counts
- Quick intuition
  - Partial derivative in logistic regression

$$\frac{\partial}{\partial \boldsymbol{\omega}_i}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = \sum_t \phi_i(\boldsymbol{x}_t, \boldsymbol{y}_t) - \sum_t \sum_{\boldsymbol{y}' \in \mathcal{Y}} P(\boldsymbol{y}'|\boldsymbol{x}_t)\phi_i(\boldsymbol{x}_t, \boldsymbol{y}')$$

  - First term is empirical feature counts and second term is expected counts
  - Derivative set to zero maximizes function
  - Therefore when both counts are equivalent, we optimize the logistic regression objective!

Perceptron

Perceptron Learning Algorithm

Training data: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

1. $\boldsymbol{\omega}^{(0)} = 0$; $i = 0$
2. for $n : 1..N$
3. for $t : 1..T$
4. Let $\boldsymbol{y}' = \arg\max_{\boldsymbol{y}'} \boldsymbol{\omega}^{(i)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
5. if $\boldsymbol{y}' \neq \boldsymbol{y}_t$
6. $\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
7. $i = i + 1$
8. return $\boldsymbol{\omega}^i$

Perceptron: Separability and Margin

- Given an training instance $(\boldsymbol{x}_t, \boldsymbol{y}_t)$, define:
  - $\bar{\mathcal{Y}}_t = \mathcal{Y} - \{\boldsymbol{y}_t\}$
  - i.e., $\bar{\mathcal{Y}}_t$ is the set of incorrect labels for $\boldsymbol{x}_t$
- A training set $\mathcal{T}$ is separable with margin $\gamma > 0$ if there exists a vector $\mathbf{u}$ with $\|\mathbf{u}\| = 1$ such that:

$$\mathbf{u} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \mathbf{u} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma \qquad (2)$$

  for all $\boldsymbol{y}' \in \bar{\mathcal{Y}}_t$ and $||\mathbf{u}|| = \sqrt{\sum_j \mathbf{u}_j^2}$
- **Assumption**: the training set is separable with margin γ

Perceptron: Main Theorem

- **Theorem**: For any training set separable with a margin of γ, the following holds for the perceptron algorithm:

  $$\text{mistakes made during training} \leq \frac{R^2}{\gamma^2}$$

  where $R \geq ||\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')||$ for all $(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$ and $\boldsymbol{y}' \in \bar{\mathcal{Y}}_t$
- Thus, after a finite number of training iterations, the error on the training set will converge to zero
- **Let's prove it!**

Perceptron Learning Algorithm

Training data: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

1. $\boldsymbol{\omega}^{(0)} = 0$; $i = 0$
2. for $n : 1..N$
3. for $t : 1..T$
4. Let $\boldsymbol{y}' = \arg\max_{\boldsymbol{y}'} \boldsymbol{\omega}^{(i)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
5. if $\boldsymbol{y}' \neq \boldsymbol{y}_t$
6. $\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
7. $i = i + 1$
8. return $\boldsymbol{\omega}^i$

- Lower bound:

  $\boldsymbol{\omega}^{(k-1)}$ are weights before k^{th} error

  Suppose k^{th} error made at $(\boldsymbol{x}_t, \boldsymbol{y}_t)$

  $\boldsymbol{y}' = \arg\max_{\boldsymbol{y}'} \boldsymbol{\omega}^{(k-1)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$

  $\boldsymbol{y}' \neq \boldsymbol{y}_t$

  $\boldsymbol{\omega}^{(k)} =$
  $\boldsymbol{\omega}^{(k-1)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$

Perceptron Learning Algorithm

Training data: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

$\boldsymbol{\omega}^{(0)} = 0$; $i = 0$
for $n : 1..N$
  for $t : 1..T$
    Let $\boldsymbol{y}' = \arg\max_{\boldsymbol{y}'} \boldsymbol{\omega}^{(i)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
    if $\boldsymbol{y}' \neq \boldsymbol{y}_t$
      $\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
      $i = i + 1$
return $\boldsymbol{\omega}^i$

- Lower bound:

  $\boldsymbol{\omega}^{(k-1)}$ are weights before k^{th} error

  Suppose k^{th} error made at $(\boldsymbol{x}_t, \boldsymbol{y}_t)$

  $\boldsymbol{y}' = \arg\max_{\boldsymbol{y}'} \boldsymbol{\omega}^{(k-1)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$

  $\boldsymbol{y}' \neq \boldsymbol{y}_t$

  $\boldsymbol{\omega}^{(k)} =$
  $\boldsymbol{\omega}^{(k-1)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$

$\mathbf{u} \cdot \boldsymbol{\omega}^{(k)} = \mathbf{u} \cdot \boldsymbol{\omega}^{(k-1)} + \mathbf{u} \cdot (\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')) \geq \mathbf{u} \cdot \boldsymbol{\omega}^{(k-1)} + \gamma$, by (2)
Since $\boldsymbol{\omega}^{(0)} = 0$ and $\mathbf{u} \cdot \boldsymbol{\omega}^{(0)} = 0$, for all k: $\mathbf{u} \cdot \boldsymbol{\omega}^{(k)} \geq k\gamma$, by induction on k
Since $\mathbf{u} \cdot \boldsymbol{\omega}^{(k)} \leq ||\mathbf{u}|| \times ||\boldsymbol{\omega}^{(k)}||$, by the law of cosines, and $||\mathbf{u}|| = 1$, then
$||\boldsymbol{\omega}^{(k)}|| \geq k\gamma$

Perceptron Learning Algorithm

Training data: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

$\boldsymbol{\omega}^{(0)} = 0; \; i = 0$
for $n : 1..N$
  for $t : 1..T$
    Let $\boldsymbol{y}' = \arg\max_{\boldsymbol{y}'} \boldsymbol{\omega}^{(i)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
    if $\boldsymbol{y}' \neq \boldsymbol{y}_t$
      $\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
      $i = i + 1$
return $\boldsymbol{\omega}^i$

- Lower bound:

  $\boldsymbol{\omega}^{(k-1)}$ are weights before k^{th} error

  Suppose k^{th} error made at $(\boldsymbol{x}_t, \boldsymbol{y}_t)$

  $\boldsymbol{y}' = \arg\max_{\boldsymbol{y}'} \boldsymbol{\omega}^{(k-1)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$

  $\boldsymbol{y}' \neq \boldsymbol{y}_t$

  $\boldsymbol{\omega}^{(k)} =$
  $\boldsymbol{\omega}^{(k-1)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$

  $\mathbf{u} \cdot \boldsymbol{\omega}^{(k)} = \mathbf{u} \cdot \boldsymbol{\omega}^{(k-1)} + \mathbf{u} \cdot (\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')) \geq \mathbf{u} \cdot \boldsymbol{\omega}^{(k-1)} + \gamma$, by (2)
  Since $\boldsymbol{\omega}^{(0)} = 0$ and $\mathbf{u} \cdot \boldsymbol{\omega}^{(0)} = 0$, for all k: $\mathbf{u} \cdot \boldsymbol{\omega}^{(k)} \geq k\gamma$, by induction on k
  Since $\mathbf{u} \cdot \boldsymbol{\omega}^{(k)} \leq ||\mathbf{u}|| \times ||\boldsymbol{\omega}^{(k)}||$, by the law of cosines, and $||\mathbf{u}|| = 1$, then
  $||\boldsymbol{\omega}^{(k)}|| \geq k\gamma$

- Upper bound:

$$
\begin{aligned}
||\boldsymbol{\omega}^{(k)}||^2 &= ||\boldsymbol{\omega}^{(k-1)}||^2 + ||\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')||^2 + 2\boldsymbol{\omega}^{(k-1)} \cdot (\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')) \\
||\boldsymbol{\omega}^{(k)}||^2 &\leq ||\boldsymbol{\omega}^{(k-1)}||^2 + R^2, \text{ since } R \geq ||\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')|| \\
&\qquad \text{and } \boldsymbol{\omega}^{(k-1)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}^{(k-1)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \leq 0 \\
&\leq kR^2 \text{ for all } k, \text{ by induction on } k
\end{aligned}
$$

Perceptron Learning Algorithm

- We have just shown that $||\omega^{(k)}|| \geq k\gamma$ and $||\omega^{(k)}||^2 \leq kR^2$
- Therefore,

$$k^2\gamma^2 \leq ||\omega^{(k)}||^2 \leq kR^2$$

- and solving for k

$$k \leq \frac{R^2}{\gamma^2}$$

- Therefore the number of errors is bounded!

Perceptron Summary

- Learns parameters of a linear model by minimizing error
- Guaranteed to find a $\boldsymbol{\omega}$ in a finite amount of time
- Perceptron is an example of an Online Learning Algorithm
  - $\boldsymbol{\omega}$ is updated based on a single training instance in isolation

$$\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$$

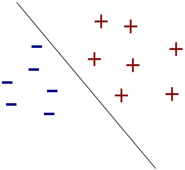
Averaged Perceptron

Training data: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

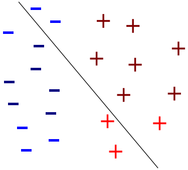
1. $\boldsymbol{\omega}^{(0)} = 0$; $i = 0$
2. for $n : 1..N$
3. for $t : 1..T$
4. Let $\boldsymbol{y}' = \arg\max_{\boldsymbol{y}'} \boldsymbol{\omega}^{(i)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
5. if $\boldsymbol{y}' \neq \boldsymbol{y}_t$
6. $\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')$
7. else
6. $\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)}$
7. $i = i + 1$
8. return $\left(\sum_i \boldsymbol{\omega}^{(i)}\right) / (N \times T)$

Margin

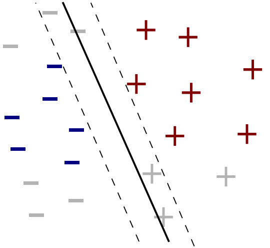
Training

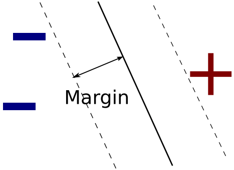


Testing



Denote the value of the margin by γ





Maximizing Margin

- For a training set $\mathcal{T}$
- Margin of a weight vector $\boldsymbol{\omega}$ is smallest γ such that

$$\boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

- for every training instance $(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$, $\boldsymbol{y}' \in \bar{\mathcal{Y}}_t$

Maximizing Margin

- Intuitively maximizing margin makes sense
- By cross-validation, the generalization error on unseen test data can be shown to be proportional to the inverse of the margin

$$\epsilon \propto \frac{R^2}{\gamma^2 \times |\mathcal{T}|}$$

- **Perceptron**: we have shown that:
  - If a training set is separable by some margin, the perceptron will find a $\boldsymbol{\omega}$ that separates the data
  - However, the perceptron does not pick $\boldsymbol{\omega}$ to maximize the margin!

Support Vector Machines (SVMs)

Maximizing Margin

Let $\gamma > 0$

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall (\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

- Note: algorithm still minimizes error if data is separable
- $||\boldsymbol{\omega}||$ is bound since scaling trivially produces larger margin

$$\beta(\boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}')) \geq \beta\gamma, \text{ for some } \beta \geq 1$$

Max Margin = Min Norm

Let $\gamma > 0$

Max Margin:

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall (\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Max Margin = Min Norm

Let $\gamma > 0$

Max Margin:

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall (\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Change variables: $\mathbf{u} = \dfrac{\boldsymbol{\omega}}{\gamma}$

$||\boldsymbol{\omega}|| = 1$ iff $||\mathbf{u}|| = 1/\gamma$, then $\gamma = 1/||\mathbf{u}||$

Max Margin = Min Norm

Let $\gamma > 0$

Max Margin:

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Change variables: $\mathbf{u} = \dfrac{\boldsymbol{\omega}}{\gamma}$

$||\boldsymbol{\omega}|| = 1$ iff $||\mathbf{u}|| = 1/\gamma$,
then $\gamma = 1/||\mathbf{u}||$

Min Norm (step 1):

$$\max_{\mathbf{u}} \quad \frac{1}{||\mathbf{u}||}$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Max Margin = Min Norm

Let $\gamma > 0$

Max Margin:

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Change variables: $\mathbf{u} = \dfrac{\boldsymbol{\omega}}{\gamma}$

$||\boldsymbol{\omega}|| = 1$ iff $||\mathbf{u}|| = 1/\gamma$,
then $\gamma = 1/||\mathbf{u}||$

Min Norm (step 1):

$$\min_{\mathbf{u}} ||\mathbf{u}||$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Max Margin = Min Norm

Let $\gamma > 0$

Max Margin:

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Change variables: $\mathbf{u} = \dfrac{\boldsymbol{\omega}}{\gamma}$

$||\boldsymbol{\omega}|| = 1$ iff $||\mathbf{u}|| = 1/\gamma$,
then $\gamma = 1/||\mathbf{u}||$

Min Norm (step 2):

$$\min_{\mathbf{u}} ||\mathbf{u}||$$

such that:

$$\gamma\mathbf{u}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \gamma\mathbf{u}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Max Margin = Min Norm

Let $\gamma > 0$

Max Margin:

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t,\boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Change variables: $\mathbf{u} = \dfrac{\boldsymbol{\omega}}{\gamma}$

$||\boldsymbol{\omega}|| = 1$ iff $||\mathbf{u}|| = 1/\gamma$,
then $\gamma = 1/||\mathbf{u}||$

Min Norm (step 2):

$$\min_{\mathbf{u}} ||\mathbf{u}||$$

such that:

$$\mathbf{u}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t) - \mathbf{u}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}') \geq 1$$

$$\forall(\boldsymbol{x}_t,\boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Max Margin = Min Norm

Let $\gamma > 0$

Max Margin:

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Change variables: $\mathbf{u} = \dfrac{\boldsymbol{\omega}}{\gamma}$

$||\boldsymbol{\omega}|| = 1$ iff $||\mathbf{u}|| = 1/\gamma$,
then $\gamma = 1/||\mathbf{u}||$

Min Norm (step 3):

$$\min_{\mathbf{u}} \quad \frac{1}{2}||\mathbf{u}||^2$$

such that:

$$\mathbf{u}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \mathbf{u}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq 1$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Max Margin = Min Norm

Let $\gamma > 0$

Max Margin:

$$\max_{||\boldsymbol{\omega}||=1} \quad \gamma$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq \gamma$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

Min Norm:

$$\min_{\mathbf{u}} \quad \frac{1}{2}||\mathbf{u}||^2$$

such that:

$$\mathbf{u}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \mathbf{u}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq 1$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$$

$$\text{and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

- Intuition: Instead of fixing $||\boldsymbol{\omega}||$ we fix the margin $\gamma = 1$

Support Vector Machines

- **Constrained Optimization Problem**

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega}} \ \frac{1}{2}||\boldsymbol{\omega}||^2$$

such that:

$$\boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq 1$$

$$\forall (\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T} \text{ and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

- **Support Vectors:** Examples where

$$\boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') = 1$$

for training instance $(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$ and all $\boldsymbol{y}' \in \bar{\mathcal{Y}}_t$

Support Vector Machines

- **What if data is not separable?**

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega},\xi} \ \frac{1}{2}||\boldsymbol{\omega}||^2 + C\sum_{t=1}^{|\mathcal{T}|}\xi_t$$

such that:

$$\boldsymbol{\omega} \cdot \phi(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega} \cdot \phi(\boldsymbol{x}_t, \boldsymbol{y}') \geq 1 - \xi_t \text{ and } \xi_t \geq 0$$

$$\forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T} \text{ and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

- ξ_t: slack variable representing amount of constraint violation
- If data is separable, optimal solution has $\xi_i = 0$, $\forall i$
  C balances focus on margin and on error

Support Vector Machines

- **What if data is not separable?**

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega},\xi} \; \frac{1}{2}||\boldsymbol{\omega}||^2 + C\sum_{t=1}^{|\mathcal{T}|}\xi_t$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}') \geq 1-\xi_t \text{ and } \xi_t \geq 0$$

$$\forall(\boldsymbol{x}_t,\boldsymbol{y}_t)\in\mathcal{T} \text{ and } \boldsymbol{y}'\in\bar{\mathcal{Y}}_t$$

- ξ_t: slack variable representing amount of constraint violation
- If data is separable, optimal solution has $\xi_i = 0$, $\forall i$
  C balances focus on margin ($C < \frac{1}{2}$) and on error ($C > \frac{1}{2}$)

Support Vector Machines

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega},\xi} \; \frac{1}{2}||\boldsymbol{\omega}||^2 + C\sum_{t=1}^{|\mathcal{T}|}\xi_t$$

such that:

$$\boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') \geq 1 - \xi_t$$
$$\text{where } \xi_t \geq 0 \text{ and } \forall(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T} \text{ and } \boldsymbol{y}' \in \bar{\mathcal{Y}}_t$$

- Computing the dual form results in a quadratic programming problem – a well-known convex optimization problem
- Can we have representation of this objective that allows more direct optimization?

Support Vector Machines

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega},\xi} \ \frac{1}{2}||\boldsymbol{\omega}||^2 + C\sum_{t=1}^{|\mathcal{T}|}\xi_t$$

such that:

$$\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t) - \max_{\boldsymbol{y}'\neq\boldsymbol{y}_t} \ \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}') \geq 1-\xi_t$$

Support Vector Machines

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega},\xi} \ \frac{1}{2}||\boldsymbol{\omega}||^2 + C\sum_{t=1}^{|\mathcal{T}|}\xi_t$$

such that:

$$\xi_t \geq 1 + \underbrace{\max_{\boldsymbol{y}' \neq \boldsymbol{y}_t} \ \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)}_{\textit{negated margin for example}}$$

Support Vector Machines

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega},\xi} \ \frac{\lambda}{2}||\boldsymbol{\omega}||^2 + \sum_{t=1}^{|\mathcal{T}|} \xi_t \qquad \lambda = \frac{1}{C}$$

such that:

$$\xi_t \geq 1 + \underbrace{\max_{\boldsymbol{y}' \neq \boldsymbol{y}_t} \ \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)}_{\textit{negated margin for example}}$$

Support Vector Machines

$$\xi_t \geq 1 + \underbrace{\max_{\boldsymbol{y}' \neq \boldsymbol{y}_t} \ \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)}_{\textit{negated margin for example}}$$

- If $\|\boldsymbol{\omega}\|$ classifies $(\boldsymbol{x}_t, \boldsymbol{y}_t)$ with margin 1, penalty $\xi_t = 0$
- Otherwise: $\xi_t = 1 + \max_{\boldsymbol{y}' \neq \boldsymbol{y}_t} \ \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)$
- That means that in the end ξ_t will be:

$$\xi_t = \max\{0, 1 + \max_{\boldsymbol{y}' \neq \boldsymbol{y}_t} \ \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)\}$$

Support Vector Machines

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega},\xi} \frac{\lambda}{2}||\boldsymbol{\omega}||^2 + \sum_{t=1}^{|\mathcal{T}|} \xi_t \text{ s.t. } \xi_t \geq 1 + \max_{\boldsymbol{y}' \neq \boldsymbol{y}_t} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)$$

Hinge loss

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega}} \mathcal{L}(\mathcal{T}; \boldsymbol{\omega}) = \arg\min_{\boldsymbol{\omega}} \sum_{t=1}^{|\mathcal{T}|} loss((\boldsymbol{x}_t, \boldsymbol{y}_t); \boldsymbol{\omega}) + \frac{\lambda}{2}||\boldsymbol{\omega}||^2$$

$$= \arg\min_{\boldsymbol{\omega}} \left(\sum_{t=1}^{|\mathcal{T}|} \max\left(0, 1 + \max_{\boldsymbol{y}' \neq \boldsymbol{y}_t} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}') - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)\right) \right) + \frac{\lambda}{2}||\boldsymbol{\omega}||^2$$

- Hinge loss allows **unconstrained optimization** (later!)

Summary

What we have covered

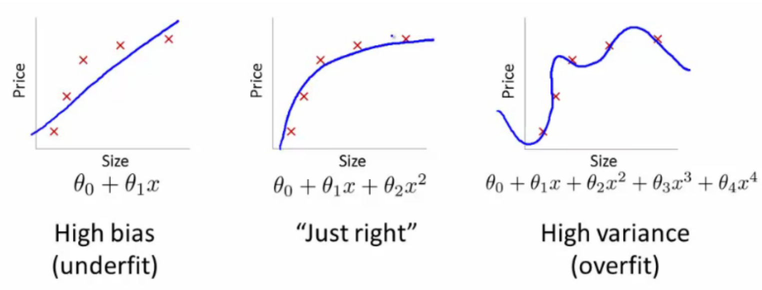
- Linear Models
  - Naive Bayes
  - Logistic Regression
  - Perceptron
  - Support Vector Machines

What is next

- Regularization
- Online learning
- Non-linear models

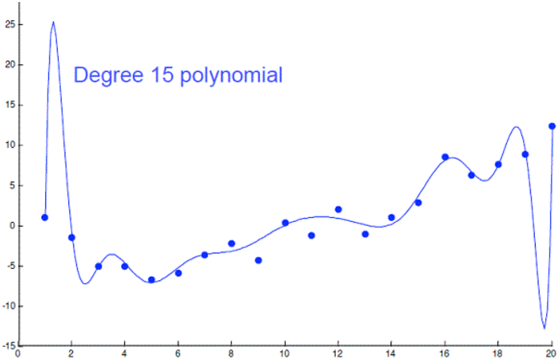
Regularization

Fit of a Model



- Two sources of error:
  - Bias error, measures how well the hypothesis class fits the space we are trying to model
  - Variance error, measures sensitivity to training set selection
  - Want to balance these two things

Fit of a Model



Overfitting

- Early in lecture we made assumption data was i.i.d.
  - Rarely is this true, e.g., syntactic analyzers typically trained on 40,000 sentences from early 1990s WSJ news text
- Even more common: $\mathcal{T}$ is very small
  - This leads to overfitting
- E.g.: 'fake' is never a verb in WSJ treebank (only adjective)
  - High weight on "$\boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}) = 1$ if $\boldsymbol{x}$=fake and $\boldsymbol{y}$=adjective"
  - Of course: leads to high log-likelihood / low error
  - Other features might be more indicative, e.g., adjacent word identities: 'He wants to X his death' $\rightarrow$ X=verb

Regularization

- In practice, we regularize models to prevent overfitting

$$\arg\max_{\boldsymbol{\omega}} \; \mathcal{L}(\mathcal{T};\boldsymbol{\omega}) - \lambda\mathcal{R}(\boldsymbol{\omega})$$

- Where $\mathcal{R}(\boldsymbol{\omega})$ is the regularization function
- λ controls how much to regularize
- Most common regularizer
  - L2: $\mathcal{R}(\boldsymbol{\omega}) \propto \|\boldsymbol{\omega}\|_2 = \|\boldsymbol{\omega}\| = \sqrt{\sum_i \omega_i^2}$ – smaller weights desired

Logistic Regression with L2 Regularization

- Perhaps most common learner in NLP

$$\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) - \lambda\mathcal{R}(\boldsymbol{\omega}) = \sum_{t=1}^{|\mathcal{T}|} \log\left(e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)}/Z_{\boldsymbol{x}}\right) - \frac{\lambda}{2}\|\boldsymbol{\omega}\|^2$$

- What are the new partial derivatives?

$$\frac{\partial}{\partial w_i}\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) - \frac{\partial}{\partial w_i}\lambda\mathcal{R}(\boldsymbol{\omega})$$

- We know $\frac{\partial}{\partial w_i}\mathcal{L}(\mathcal{T};\boldsymbol{\omega})$
- Just need $\frac{\partial}{\partial w_i}\frac{\lambda}{2}\|\boldsymbol{\omega}\|^2 = \frac{\partial}{\partial w_i}\frac{\lambda}{2}\left(\sqrt{\sum_i \boldsymbol{\omega}_i^2}\right)^2 = \frac{\partial}{\partial w_i}\frac{\lambda}{2}\sum_i \boldsymbol{\omega}_i^2 = \lambda\boldsymbol{\omega}_i$

Support Vector Machines

- SVM in hinge-loss formulation: L2 regularization corresponds to margin maximization!

$$\boldsymbol{\omega} \quad = \quad \arg\min_{\boldsymbol{\omega}} \; \mathcal{L}(\mathcal{T}; \boldsymbol{\omega}) + \lambda \mathcal{R}(\boldsymbol{\omega})$$

Support Vector Machines

- SVM in hinge-loss formulation: L2 regularization corresponds to margin maximization!

$$
\begin{aligned}
\boldsymbol{\omega} &= \arg\min_{\boldsymbol{\omega}} \; \mathcal{L}(\mathcal{T}; \boldsymbol{\omega}) + \lambda \mathcal{R}(\boldsymbol{\omega}) \\
&= \arg\min_{\boldsymbol{\omega}} \; \sum_{t=1}^{|\mathcal{T}|} \mathit{loss}((\boldsymbol{x}_t, \boldsymbol{y}_t); \boldsymbol{\omega}) + \lambda \mathcal{R}(\boldsymbol{\omega})
\end{aligned}
$$

Support Vector Machines

- SVM in hinge-loss formulation: L2 regularization corresponds to margin maximization!

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\boldsymbol{\omega} &= \arg\min_{\boldsymbol{\omega}} \; \mathcal{L}(\mathcal{T}; \boldsymbol{\omega}) + \lambda \mathcal{R}(\boldsymbol{\omega}) \\
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&= \arg\min_{\boldsymbol{\omega}} \; \sum_{t=1}^{|\mathcal{T}|} \max\left(0, 1 + \max_{\boldsymbol{y} \neq \boldsymbol{y}_t} \; \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)\right) + \lambda \mathcal{R}(\boldsymbol{\omega})
\end{aligned}
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&= \arg\min_{\boldsymbol{\omega}} \sum_{t=1}^{|\mathcal{T}|} \max\left(0, 1 + \max_{\boldsymbol{y} \neq \boldsymbol{y}_t} \ \boldsymbol{\omega}\cdot\phi(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\omega}\cdot\phi(\boldsymbol{x}_t, \boldsymbol{y}_t)\right) + \lambda\mathcal{R}(\boldsymbol{\omega}) \\
&= \arg\min_{\boldsymbol{\omega}} \sum_{t=1}^{|\mathcal{T}|} \max\left(0, 1 + \max_{\boldsymbol{y} \neq \boldsymbol{y}_t} \ \boldsymbol{\omega}\cdot\phi(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\omega}\cdot\phi(\boldsymbol{x}_t, \boldsymbol{y}_t)\right) + \frac{\lambda}{2}\|\boldsymbol{\omega}\|^2
\end{aligned}
$$

SVMs vs. Logistic Regression

$$
\begin{aligned}
\boldsymbol{\omega} &= \arg\min_{\boldsymbol{\omega}} \; \mathcal{L}(\mathcal{T};\boldsymbol{\omega}) + \lambda\mathcal{R}(\boldsymbol{\omega}) \\
&= \arg\min_{\boldsymbol{\omega}} \; \sum_{t=1}^{|\mathcal{T}|} \mathit{loss}((\boldsymbol{x}_t, \boldsymbol{y}_t);\boldsymbol{\omega}) + \lambda\mathcal{R}(\boldsymbol{\omega})
\end{aligned}
$$

SVMs vs. Logistic Regression

$$\begin{aligned}\boldsymbol{\omega} &= \arg\min_{\boldsymbol{\omega}} \; \mathcal{L}(\mathcal{T};\boldsymbol{\omega}) + \lambda\mathcal{R}(\boldsymbol{\omega}) \\ &= \arg\min_{\boldsymbol{\omega}} \; \sum_{t=1}^{|\mathcal{T}|} \mathit{loss}((\boldsymbol{x}_t,\boldsymbol{y}_t);\boldsymbol{\omega}) + \lambda\mathcal{R}(\boldsymbol{\omega})\end{aligned}$$

SVMs/hinge-loss: $\max\,(0, 1 + \max_{\boldsymbol{y}\neq\boldsymbol{y}_t}\,(\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)))$

$$\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega}} \sum_{t=1}^{|\mathcal{T}|} \max\,(0, 1 + \max_{\boldsymbol{y}\neq\boldsymbol{y}_t}\; \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)) + \frac{\lambda}{2}\|\boldsymbol{\omega}\|^2$$

SVMs vs. Logistic Regression

$$
\begin{aligned}
\boldsymbol{\omega} &= \arg\min_{\boldsymbol{\omega}} \; \mathcal{L}(\mathcal{T};\boldsymbol{\omega}) + \lambda\mathcal{R}(\boldsymbol{\omega}) \\
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\end{aligned}
$$

SVMs/hinge-loss: $\max\left(0, 1 + \max_{\boldsymbol{y}\neq\boldsymbol{y}_t}\left(\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)\right)\right)$

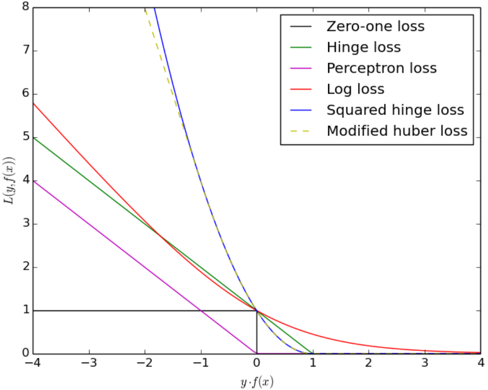
$$
\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega}} \sum_{t=1}^{|\mathcal{T}|} \max\left(0, 1 + \max_{\boldsymbol{y}\neq\boldsymbol{y}_t} \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}) - \boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)\right) + \frac{\lambda}{2}\|\boldsymbol{\omega}\|^2
$$

Logistic Regression/log-loss: $-\log\left(e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)}/Z_{\boldsymbol{x}}\right)$

$$
\boldsymbol{\omega} = \arg\min_{\boldsymbol{\omega}} \sum_{t=1}^{|\mathcal{T}|} -\log\left(e^{\boldsymbol{\omega}\cdot\boldsymbol{\phi}(\boldsymbol{x}_t,\boldsymbol{y}_t)}/Z_{\boldsymbol{x}}\right) + \frac{\lambda}{2}\|\boldsymbol{\omega}\|^2
$$

Summary: Loss Functions

$$\omega = \arg\min_{\omega} \; \mathcal{L}(\mathcal{T};\omega) + \lambda\mathcal{R}(\omega) = \arg\min_{\omega} \; \sum_{t=1}^{|\mathcal{T}|} \mathit{loss}((\boldsymbol{x}_t, \boldsymbol{y}_t);\omega) + \lambda\mathcal{R}(\omega)$$



Online Learning

Online vs. Batch Learning

Batch($\mathcal{T}$);

- for 1 ... N
  - $\boldsymbol{\omega} \leftarrow$ update($\mathcal{T}; \boldsymbol{\omega}$)
- return $\boldsymbol{\omega}$

E.g., SVMs, logistic regression, Naive Bayes

Online($\mathcal{T}$);

- for 1 ... N
  - for $(\boldsymbol{x}_t, \boldsymbol{y}_t) \in \mathcal{T}$
    - $\boldsymbol{\omega} \leftarrow$ update($(\boldsymbol{x}_t, \boldsymbol{y}_t); \boldsymbol{\omega}$)
  - end for
- end for
- return $\boldsymbol{\omega}$

E.g., Perceptron

$$\boldsymbol{\omega} = \boldsymbol{\omega} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y})$$

Batch Gradient Descent

- Let $\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = \sum_{t=1}^{|\mathcal{T}|} loss((\boldsymbol{x}_t, \boldsymbol{y}_t);\boldsymbol{\omega})$
  - Set $\boldsymbol{\omega}^0 = O^m$
  - Iterate until convergence

$$
\begin{aligned}
\boldsymbol{\omega}^i &= \boldsymbol{\omega}^{i-1} - \alpha \nabla \mathcal{L}(\mathcal{T};\boldsymbol{\omega}^{i-1}) \\
&= \boldsymbol{\omega}^{i-1} - \sum_{t=1}^{|\mathcal{T}|} \alpha \nabla loss((\boldsymbol{x}_t, \boldsymbol{y}_t);\boldsymbol{\omega}^{i-1})
\end{aligned}
$$

- $\alpha > 0$ and set so that $\mathcal{L}(\mathcal{T};\boldsymbol{\omega}^i) < \mathcal{L}(\mathcal{T};\boldsymbol{\omega}^{i-1})$

Stochastic Gradient Descent

- Stochastic Gradient Descent (SGD)
  - Approximate batch gradient $\nabla\mathcal{L}(\mathcal{T};\boldsymbol{\omega})$ with stochastic gradient $\nabla loss((\boldsymbol{x}_t,\boldsymbol{y}_t);\boldsymbol{\omega})$
- Let $\mathcal{L}(\mathcal{T};\boldsymbol{\omega}) = \sum_{t=1}^{|\mathcal{T}|} loss((\boldsymbol{x}_t,\boldsymbol{y}_t);\boldsymbol{\omega})$
  - Set $\boldsymbol{\omega}^0 = O^m$
  - iterate until convergence
    - sample $(\boldsymbol{x}_t,\boldsymbol{y}_t) \in \mathcal{T}$ // "stochastic"
    - $\boldsymbol{\omega}^i = \boldsymbol{\omega}^{i-1} - \alpha\nabla loss((\boldsymbol{x}_t,\boldsymbol{y}_t);\boldsymbol{\omega}^{i-1})$
  - return $\boldsymbol{\omega}$

Online Logistic Regression

- Stochastic Gradient Descent (SGD)
- $\textit{loss}((\boldsymbol{x}_t, \boldsymbol{y}_t); \boldsymbol{\omega})$ = log-loss
- $\nabla \textit{loss}((\boldsymbol{x}_t, \boldsymbol{y}_t); \boldsymbol{\omega}) = \nabla \left(-\log \left(e^{\boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)} / Z_{\boldsymbol{x}_t} \right) \right)$
- From logistic regression section:

$$\nabla \left(-\log \left(e^{\boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)} / Z_{\boldsymbol{x}_t} \right) \right) = - \left(\phi(\boldsymbol{x}_t, \boldsymbol{y}_t) - \sum_{\boldsymbol{y}} P(\boldsymbol{y}|\boldsymbol{x}) \phi(\boldsymbol{x}_t, \boldsymbol{y}) \right)$$

- Plus regularization term (if part of model)

Online SVMs

- Stochastic Gradient Descent (SGD)
- $\mathit{loss}((\boldsymbol{x}_t, \boldsymbol{y}_t); \boldsymbol{\omega}) = \text{hinge-loss}$

$$\nabla \mathit{loss}((\boldsymbol{x}_t, \boldsymbol{y}_t); \boldsymbol{\omega}) = \nabla \left(\max\left(0, 1 + \max_{\boldsymbol{y} \neq \boldsymbol{y}_t} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)\right) \right)$$

- Subgradient is:

$$\nabla \left(\max\left(0, 1 + \max_{\boldsymbol{y} \neq \boldsymbol{y}_t} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)\right) \right)$$

$$= \begin{cases} 0, & \text{if } \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \max_{\boldsymbol{y}} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) \geq 1 \\ \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t), & \text{otherwise, where } \boldsymbol{y} = \max_{\boldsymbol{y}} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) \end{cases}$$

- Plus regularization term (L2 norm for SVMs):

$$\nabla \frac{\lambda}{2} ||\boldsymbol{\omega}||^2 = \lambda \boldsymbol{\omega}$$

Perceptron and Hinge-Loss

SVM subgradient update looks like perceptron update

$$\boldsymbol{\omega}^{i} = \boldsymbol{\omega}^{i-1} - \alpha \begin{cases} \lambda \boldsymbol{\omega}, & \text{if } \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \max_{\boldsymbol{y}} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) \geq 1 \\ \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) + \lambda \boldsymbol{\omega}, & \text{otherwise, where } \boldsymbol{y} = \max_{\boldsymbol{y}} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) \end{cases}$$

Perceptron

$$\boldsymbol{\omega}^{i} = \boldsymbol{\omega}^{i-1} - \alpha \begin{cases} 0, & \text{if } \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \max_{\boldsymbol{y}} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) \geq 0 \\ \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t), & \text{otherwise, where } \boldsymbol{y} = \max_{\boldsymbol{y}} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) \end{cases}$$

Perceptron = SGD optimization of no-margin hinge-loss (without regularization):

$$\max\left(0, 1 + \max_{\boldsymbol{y} \neq \boldsymbol{y}_t} \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) - \boldsymbol{\omega} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)\right)$$

Online vs. Batch Learning

- Online algorithms
  - Each update step relies only on the derivative for a single randomly chosen example
    - Computational cost of one step is $1/\mathcal{T}$ compared to batch
    - Easier to implement
  - Larger variance since each gradient is different
    - Variance slows down convergence
    - Requires fine-tuning of decaying learning rate
- Batch algorithms
  - Higher cost of averaging gradients over $\mathcal{T}$ for each update
    - Implementation more complex
    - Less fine-tuning, e.g., allows constant learning rates
    - Faster convergence

Variance-Reduced Online Learning

- SGD update extended by velocity vector $\boldsymbol{v}$ weighted by momentum coefficient $0 \leq \mu < 1$ [Polyak 1964]:
  - $$\boldsymbol{\omega}^{i+1} = \boldsymbol{\omega}^{i} - \alpha \nabla \mathit{loss}((\boldsymbol{x}_t, \boldsymbol{y}_t); \boldsymbol{\omega}^{i}) + \mu \boldsymbol{v}^{i}$$

    where

    $$\boldsymbol{v}^{i} = \boldsymbol{\omega}^{i} - \boldsymbol{\omega}^{i-1}$$
  - Momentum accelerates learning if gradients are aligned along same direction, and restricts changes when successive gradient are opposite of each other
  - General direction of gradient reinforced, perpendicular directions filtered out
- Best of both worlds: Efficient and effective!

Online-to-Batch Conversion

- Classical online learning:
  - data are given as an infinite sequence of input examples
  - model makes prediction on next example in sequence
- Standard NLP applications:
  - finite set of training data, prediction on new batch of test data
  - online learning applied by cycling over finite data
  - online-to-batch conversion: Which model to use at test time?
    - Last model? Random model? Best model on heldout set?

Online-to-Batch Conversion by Averaging

- Averaged Perceptron
  - $\bar{\boldsymbol{\omega}} = \left(\sum_i \boldsymbol{\omega}^{(i)}\right) / (N \times T)$
  - Use weight vector averaged over online updates for prediction
- How does the perceptron mistake bound carry over to batch?
  - Let M_K be number of mistakes made during online learning, then with probability of at least $1 - \delta$:

$$\mathbb{E}[loss((\boldsymbol{x}, \boldsymbol{y}); \bar{\boldsymbol{\omega}})] \leq M_k + \sqrt{\frac{2}{k} \ln \frac{1}{\delta}}$$

  - $=$ generalization bound based on online performance [Cesa-Bianchi et al. 2004]
  - can be applied to all online learners with convex losses

Quick Summary

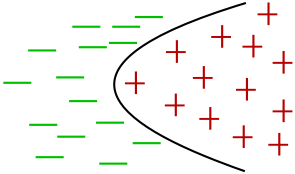
Linear Learners

- Naive Bayes, Perceptron, Logistic Regression and SVMs
- Objective functions and loss functions
- Convex Optimization
- Regularization
- Online vs. Batch learning

Non-Linear Models

Non-Linear Models

- Some data sets require more than a linear decision boundary to be correctly modeled
- Decision boundary is no longer a hyperplane in the feature space



Kernel Machines = Convex Optimization for Non-Linear Models

- Projecting a linear model into a higher dimensional feature space can correspond to a non-linear model in the original space and make non-separable problems separable
- For classifiers based on similarity functions (= kernels), computing a non-linear kernel is often more efficient than calculating the corresponding dot product in the high dimensional feature space
- Thus, kernels allow us to efficiently learn non-linear models by convex optimization

Monomial Features and Polynomial Kernels

- Monomial features = d^{th} order products of entries x_j of $\boldsymbol{x}$ s.t. $x_{j_1} * x_{j_2} * \cdots * x_{j_d}$ for $j_1, \ldots, j_d \in \{1 \ldots n\}$
- Ordered monomial feature map: $\phi : \mathbb{R}^2 \to \mathbb{R}^4$ s.t. $(x_1, x_2) \mapsto (x_1^2, x_2^2, x_1x_2, x_2x_1)$
- Computation of kernel from feature map:

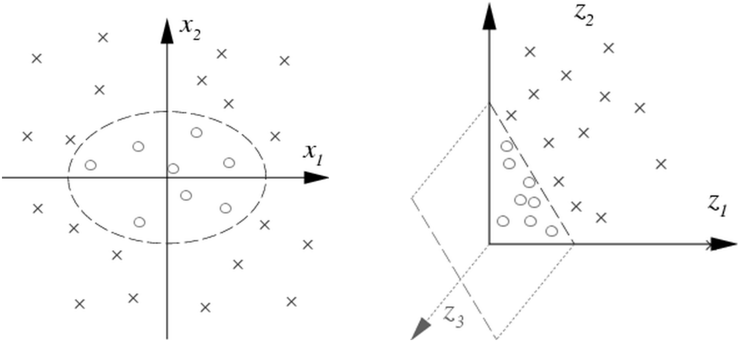
$$\begin{aligned}
\phi(\boldsymbol{x}) \cdot \phi(\boldsymbol{x}') &= \sum_{i=1}^{4} \phi_i(\boldsymbol{x})\phi_i(\boldsymbol{x}') \text{ (Def. dot product)} \\
&= x_1^2 {x'}_1^2 + x_2^2 {x'}_2^2 + x_1x_2{x'}_1{x'}_2 + x_2x_1{x'}_2{x'}_1 \text{ (Def. } \phi\text{)} \\
&= x_1^2 {x'}_1^2 + x_2^2 {x'}_2^2 + 2x_1x_2{x'}_1{x'}_2 \\
&= \left(x_1{x'}_1 + x_2{x'}_2\right)^2
\end{aligned}$$

- Direct application of kernel: $\phi(\boldsymbol{x}) \cdot \phi(\boldsymbol{x}') = (\boldsymbol{x} \cdot \boldsymbol{x}')^2$

Direct Application of Kernel

- Let C_d be a map from $\boldsymbol{x} \in \mathbb{R}^m$ to vectors $C_d(\boldsymbol{x})$ of all d^{th}-degree ordered products of entries of $\boldsymbol{x}$.
  Then the corresponding kernel computing the dot product of vectors mapped by C_d is:
  $K(\boldsymbol{x}, \boldsymbol{x}') = C_d(\boldsymbol{x}) \cdot C_d(\boldsymbol{x}') = (\boldsymbol{x} \cdot \boldsymbol{x}')^d$
- Alternative feature map satisfying this definition = unordered monomial: $\phi_2 : \mathbb{R}^2 \to \mathbb{R}^3$ s.t. $(x_1, x_2) \mapsto (x_1^2, x_2^2, \sqrt{2}x_1x_2)$

Non-Linear Feature Map



$$\phi_2 : \mathbb{R}^2 \rightarrow \mathbb{R}^3 \text{ s.t. } (x_1, x_2) \mapsto (z_1, z_2, z_3) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

Kernel Definition

- A kernel is a similarity function between two points that is symmetric and positive definite, which we denote by:

$$K(\boldsymbol{x}_t, \boldsymbol{x}_r) \in \mathbb{R}$$

- Let M be a $n \times n$ matrix such that ...

$$M_{t,r} = K(\boldsymbol{x}_t, \boldsymbol{x}_r)$$

- ... for any n points. Called the Gram matrix.
- Symmetric:

$$K(\boldsymbol{x}_t, \boldsymbol{x}_r) = K(\boldsymbol{x}_r, \boldsymbol{x}_t)$$

- Positive definite: positivity on diagonal

$$K(\boldsymbol{x}, \boldsymbol{x}) \geq 0 \text{ forall } \boldsymbol{x} \text{ with equality only for } \boldsymbol{x} = 0$$

Mercer's Theorem

- **Mercer's Theorem**: for any kernel K, there exists a ϕ in some $\mathbb{R}^d$, such that:

$$K(\boldsymbol{x}_t, \boldsymbol{x}_r) = \boldsymbol{\phi}(\boldsymbol{x}_t) \cdot \boldsymbol{\phi}(\boldsymbol{x}_r)$$

- This means that instead of mapping input data via non-lineear feature map ϕ and then computing dot product, we can apply kernels directly *without even knowing about* ϕ!

Kernel Trick

- Define a kernel, and do not explicitly use dot product between vectors, only kernel calculations
- In some high-dimensional space, this corresponds to dot product
- In that space, the decision boundary is linear, but in the original space, we now have a non-linear decision boundary

Kernel Trick

- Define a kernel, and do not explicitly use dot product between vectors, only kernel calculations
- In some high-dimensional space, this corresponds to dot product
- In that space, the decision boundary is linear, but in the original space, we now have a non-linear decision boundary
- Note: Since our features are over pairs $(\boldsymbol{x}, \boldsymbol{y})$, we will write kernels over pairs

$$K((\boldsymbol{x}_t, \boldsymbol{y}_t), (\boldsymbol{x}_r, \boldsymbol{y}_r)) = \phi(\boldsymbol{x}_t, \boldsymbol{y}_t) \cdot \phi(\boldsymbol{x}_r, \boldsymbol{y}_r)$$

- Let's do it for the Perceptron!

Kernel Trick – Perceptron Algorithm

Training data: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

1. $\boldsymbol{\omega}^{(0)} = 0$; $i = 0$
2. for $n : 1..N$
3. for $t : 1..T$
4. Let $\boldsymbol{y} = \arg\max_{\boldsymbol{y}} \boldsymbol{\omega}^{(i)} \cdot \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y})$
5. if $\boldsymbol{y} \neq \boldsymbol{y}_t$
6. $\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y})$
7. $i = i + 1$
8. return $\boldsymbol{\omega}^i$

Kernel Trick – Perceptron Algorithm

Training data: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

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7. $i = i + 1$
8. return $\boldsymbol{\omega}^{i}$

- Each feature function $\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)$ is added and $\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y})$ is subtracted to $\boldsymbol{\omega}$ say $\alpha_{\boldsymbol{y},t}$ times
  - $\alpha_{\boldsymbol{y},t}$ is proportional to the # of times during learning label $\boldsymbol{y}$ is predicted for example t and caused an update because of misclassification

Kernel Trick – Perceptron Algorithm

Training data: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

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6. $\boldsymbol{\omega}^{(i+1)} = \boldsymbol{\omega}^{(i)} + \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y})$
7. $i = i + 1$
8. return $\boldsymbol{\omega}^i$

- Each feature function $\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t)$ is added and $\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y})$ is subtracted to $\boldsymbol{\omega}$ say $\alpha_{\boldsymbol{y},t}$ times
  - $\alpha_{\boldsymbol{y},t}$ is proportional to the # of times during learning label $\boldsymbol{y}$ is predicted for example t and caused an update because of misclassification
- Thus,

$$\boldsymbol{\omega} = \sum_{t,\boldsymbol{y}} \alpha_{\boldsymbol{y},t} [\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y})]$$

Kernel Trick – Perceptron Algorithm

- We can re-write the argmax function as:

$$
\begin{aligned}
\boldsymbol{y}* &= \arg\max_{\boldsymbol{y}^*} \boldsymbol{\omega}^{(i)} \cdot \boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}^*) \\
&= \arg\max_{\boldsymbol{y}^*} \sum_{t,\boldsymbol{y}} \alpha_{\boldsymbol{y},t} [\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y})] \cdot \boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}^*) \\
&= \arg\max_{\boldsymbol{y}^*} \sum_{t,\boldsymbol{y}} \alpha_{\boldsymbol{y},t} [\boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}_t) \cdot \boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}^*) - \boldsymbol{\phi}(\boldsymbol{x}_t, \boldsymbol{y}) \cdot \boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}^*)] \\
&= \arg\max_{\boldsymbol{y}^*} \sum_{t,\boldsymbol{y}} \alpha_{\boldsymbol{y},t} [K((\boldsymbol{x}_t, \boldsymbol{y}_t), (\boldsymbol{x}, \boldsymbol{y}^*)) - K((\boldsymbol{x}_t, \boldsymbol{y}), (\boldsymbol{x}, \boldsymbol{y}^*))]
\end{aligned}
$$

- We can then re-write the perceptron algorithm strictly with kernels

Kernel Trick – Perceptron Algorithm

- Training: $\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{|\mathcal{T}|}$

1. $\forall \boldsymbol{y}, t$ set $\alpha_{\boldsymbol{y},t} = 0$
2. for $n : 1..N$
3. for $t : 1..T$
4. Let $\boldsymbol{y}^* = \arg\max_{\boldsymbol{y}^*} \sum_{t,\boldsymbol{y}} \alpha_{\boldsymbol{y},t}[K((\boldsymbol{x}_t, \boldsymbol{y}_t), (\boldsymbol{x}_t, \boldsymbol{y}^*)) - K((\boldsymbol{x}_t, \boldsymbol{y}), (\boldsymbol{x}_t, \boldsymbol{y}^*))]$
5. if $\boldsymbol{y}^* \neq \boldsymbol{y}_t$
6. $\alpha_{\boldsymbol{y}^*,t} = \alpha_{\boldsymbol{y}^*,t} + 1$

- Testing on unseen instance $\boldsymbol{x}$:

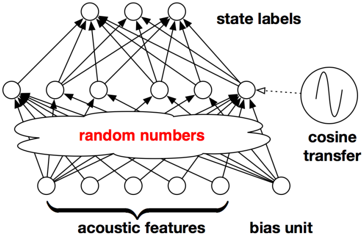
$$\boldsymbol{y}^* = \arg\max_{\boldsymbol{y}^*} \sum_{t,\boldsymbol{y}} \alpha_{\boldsymbol{y},t}[K((\boldsymbol{x}_t, \boldsymbol{y}_t), (\boldsymbol{x}, \boldsymbol{y}^*)) - K((\boldsymbol{x}_t, \boldsymbol{y}), (\boldsymbol{x}, \boldsymbol{y}^*))]$$

Kernels Summary

- Can turn a linear model into a non-linear model
- Kernels project feature space to higher dimensions
  - Sometimes exponentially larger
  - Sometimes an infinite space!
- Can “kernelize” algorithms to make them non-linear
- Convex optimization methods still applicable to learn parameters
- Disadvantage: Exact kernel methods depend polynomially on the number of training examples - infeasible for large datasets

Kernels for Large Training Sets

- Alternative to exact kernels: Explicit randomized feature map [Rahimi and Recht 2007]
  - Shallow neural network by random Fourier/Binning transformation:
    - Random weights from input to hidden units
    - Cosine as transfer function
    - Convex optimization of weights from hidden to output units



Summary

Basic principles of machine learning:

- To do learning, we set up an objective function that tells the fit of the model to the data
- We optimize with respect to the model (weights, probability model, etc.)
- Can do it in a batch or online (preferred!) fashion

What model to use?

- One example of a model: linear model
- Can kernelize/randomize these models to get non-linear models
- Convex optimization applicable for both types of model

Outlook

- Multiclass linear models are basic building blocks for further lectures: structured output prediction, graphical models, multilayer perceptron neural networks

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- Multiclass linear models are basic building blocks for further lectures: structured output prediction, graphical models, multilayer perceptron neural networks
- Kernel Machines
  - Kernel Machines introduce nonlinearity by using specific feature maps or kernels
  - Feature map or kernel is not part of optimization problem, thus convex optimization of loss function for linear model possible
- Neural Networks
  - Similarities and nonlinear combinations of features are learned: representation learning
  - We lose the advantages of convex optimization since objective functions will be nonconvex

Wrap up and time for questions

Further Reading

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