Logistic Regression

Logistic Regression

- Idea:
- Naïve Bayes allows computing P(Y|X) by learning P(Y) and P(X|Y)
- Why not learn P(Y|X) directly?

- Consider learning f: X → Y, where
  - X is a vector of real-valued features, $<X_1 \dots X_n>$
  - Y is boolean
  - assume all X_i are conditionally independent given Y
  - model $P(X_i \mid Y = y_k)$ as Gaussian $N(\mu_{ik},\sigma_i)$
  - model P(Y) as Bernoulli (π)
- What does that imply about the form of P(Y|X)?

$$P(Y=1|X=<X_1,...X_n>) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

Derive form for P(Y|X) for continuous X_i

$$\boxed{P(Y=1|X)} = \frac{P(Y=1)P(X|Y=1)}{P(Y=1)P(X|Y=1)+P(Y=0)P(X|Y=0)}$$

div by $P(Y=1)P(X|Y=1)$

$$= \frac{1}{1+\frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)}}$$

$\pi = \hat{P}(Y=1)$

$$= \frac{1}{1+\exp\left(\ln\frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)}\right)}$$

$$= \frac{1}{1+\exp\left(\left(\ln\frac{1-\pi}{\pi}\right)+\boxed{\sum_i \ln\frac{P(X_i|Y=0)}{P(X_i|Y=1)}}\right)}$$

$$P(x \mid y_k) = \frac{1}{\sigma_{ik}\sqrt{2\pi}}\, e^{\frac{-(x-\mu_{ik})^2}{2\sigma_{ik}^2}}$$

$$\boxed{\sum_i\left(\frac{\mu_{i0}-\mu_{i1}}{\sigma_i^2}X_i+\frac{\mu_{i1}^2-\mu_{i0}^2}{2\sigma_i^2}\right)}$$

$$P(Y=1|X) = \frac{1}{1+\exp(w_0+\sum_{i=1}^n w_iX_i)}$$

Very convenient!

$$P(Y=1|X=<X_1,...X_n>) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

$$P(Y=0|X=<X_1,...X_n>) =$$

implies

$$\frac{P(Y=0|X)}{P(Y=1|X)} =$$

implies

$$\ln \frac{P(Y=0|X)}{P(Y=1|X)} =$$

Very convenient!

$$P(Y=1|X=<X_1,...X_n>) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

$1 - \uparrow =$

implies

$$P(Y=0|X=<X_1,...X_n>) = \frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

$$1 \lesseqgtr \frac{P(Y=0|X)}{P(Y=1|X)} = exp(w_0 + \sum_i w_i X_i)$$

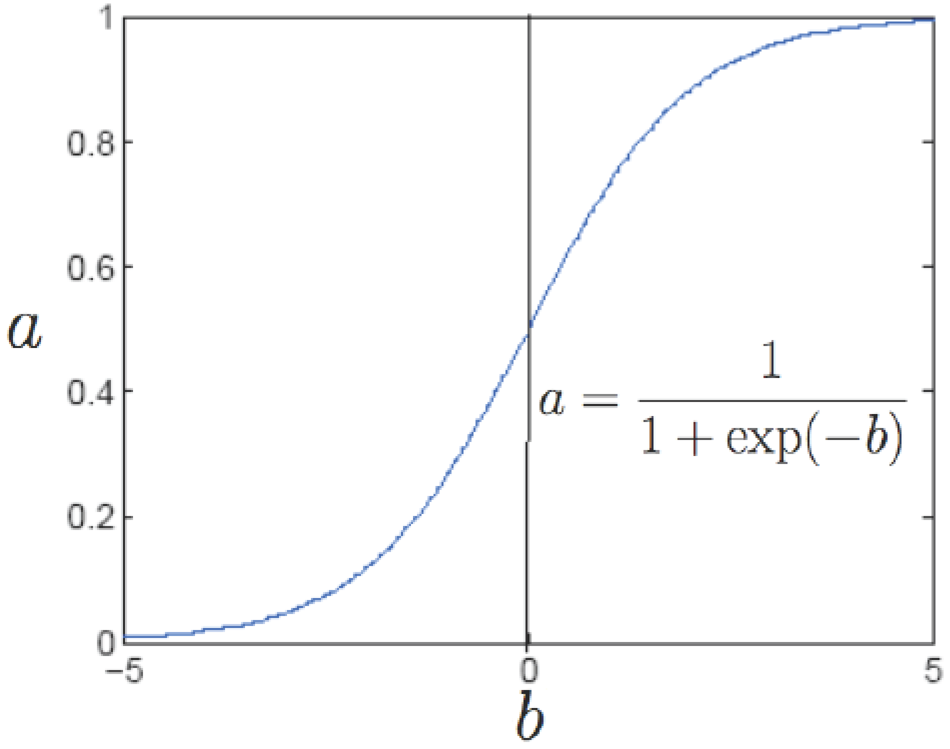
linear classification rule!

implies

$$0 \lesseqgtr \ln \frac{P(Y=0|X)}{P(Y=1|X)} = w_0 + \sum_i w_i X_i$$

log linear

Logistic function



$$\overbrace{P(Y=1|X)}^{a} = \frac{1}{1+\exp(\underbrace{w_0 + \sum_{i=1}^{n} w_i X_i}_{b})}$$

Logistic regression more generally

- Logistic regression in more general case, where $y \in \{y_1 \ldots y_R\}$: learn R-1 sets of weights

for $k<R$

$$P(Y = y_k|X) = \frac{\exp(w_{k0} + \sum_{i=1}^{n} w_{ki} X_i)}{1 + \sum_{j=1}^{R-1} \exp(w_{j0} + \sum_{i=1}^{n} w_{ji} X_i)}$$

for $k=R$

$$P(Y = y_R|X) = \frac{1}{1 + \sum_{j=1}^{R-1} \exp(w_{j0} + \sum_{i=1}^{n} w_{ji} X_i)}$$

Training Logistic Regression: MCLE

- we have L training examples: $\{\langle X^1, Y^1\rangle, \ldots \langle X^L, Y^L\rangle\}$

- maximum likelihood estimate for parameters W

$$W_{MLE} = \arg\max_W P(<X^1, Y^1> \ldots <X^L, Y^L> |W)$$
$$= \arg\max_W \prod_l P(<X^l, Y^l> |W)$$

- maximum conditional likelihood estimate

$$MCLE = \arg\max_w \prod_l P(Y^l | X^l w)$$

Training Logistic Regression: MCLE

- Choose parameters W=<w_0, ... w_n> to <u>maximize conditional likelihood</u> of training data

  where
$$P(Y=0|X,W) = \frac{1}{1+exp(w_0 + \sum_i w_i X_i)}$$
$$P(Y=1|X,W) = \frac{exp(w_0 + \sum_i w_i X_i)}{1+exp(w_0 + \sum_i w_i X_i)}$$

- Training data D = $\{\langle X^1, Y^1 \rangle, \ldots \langle X^L, Y^L \rangle\}$
- Data likelihood = $\prod_l P(X^l, Y^l | W)$
- Data conditional likelihood = $\prod_l P(Y^l | X^l, W)$

$$W_{MCLE} = \arg\max_W \prod_l P(Y^l | W, X^l)$$

Expressing Conditional Log Likelihood

$$\underline{l(W)} \equiv \underbrace{\ln \prod_l P(Y^l|X^l, W)} = \underbrace{\sum_l \ln P(Y^l|X^l, W)}$$

$$P(Y=0|X,W) = \frac{1}{1 + exp(w_0 + \sum_i w_i X_i)}$$

$$P(Y=1|X,W) = \frac{exp(w_0 + \sum_i w_i X_i)}{1 + exp(w_0 + \sum_i w_i X_i)}$$

$$\begin{aligned} l(W) &= \sum_l Y^l \ln P(Y^l = 1|X^l, W) + (1 - Y^l) \ln P(Y^l = 0|X^l, W) \\ &= \sum_l Y^l \ln \frac{P(Y^l = 1|X^l, W)}{P(Y^l = 0|X^l, W)} + \ln P(Y^l = 0|X^l, W) \\ &= \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l)) \end{aligned}$$

Maximizing Conditional Log Likelihood

$$P(Y=0|X,W) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

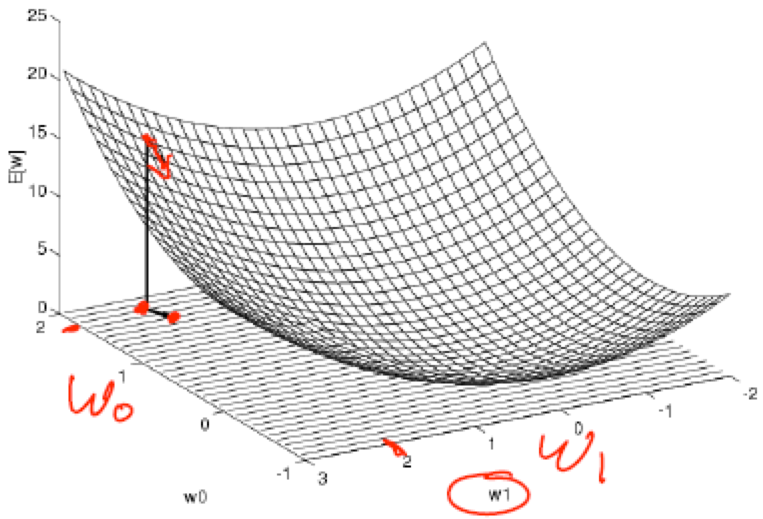
$$P(Y=1|X,W) = \frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

$$\begin{aligned} l(W) &\equiv \ln \prod_l P(Y^l|X^l,W) \\ &= \sum_l Y^l(w_0+\sum_i^n w_i X_i^l) - \ln(1+exp(w_0+\sum_i^n w_i X_i^l)) \end{aligned}$$

Good news: *l(W)* is concave function of *W*
Bad news: no closed-form solution to maximize *l(W)*

Gradient Descent

$E = \ell(w)$



Gradient

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n}\right]$$

Training rule:

$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

Maximize Conditional Log Likelihood: Gradient Ascent

$$
\begin{aligned}
l(W) &\equiv \ln \prod_l P(Y^l | X^l, W) \\
&= \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l))
\end{aligned}
$$

$$\frac{\partial l(W)}{\partial w_i} = \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))$$

Gradient ascent algorithm: iterate until change < ε

For all i,

repeat

$$w_i \leftarrow w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))$$

That’s all for M(C)LE. How about MAP?

- One common approach is to define priors on W
  - Normal distribution, zero mean, identity covariance

- Helps avoid very large weights and overfitting

- MAP estimate

$$W \leftarrow \arg\max_{W} \ln P(W) \prod_{l} P(Y^l | X^l, W)$$

- • let’s assume Gaussian prior: W ~ N(0, σ)

MLE vs MAP

- Maximum conditional likelihood estimate

$$W \leftarrow \arg\max_W \ \ln \prod_l P(Y^l | X^l, W)$$

$$\boxed{w_i \leftarrow w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))}$$

- Maximum a posteriori estimate with prior W~N(0,σI)

$$W \leftarrow \arg\max_W \ \ln[P(W) \ \prod_l \hat{P}(Y^l | X^l, W)]$$

$$\boxed{w_i \leftarrow w_i - \eta\lambda w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))}$$

MAP estimates and Regularization

- Maximum a posteriori estimate with prior W~N(0,σI)

$$W \leftarrow \arg\max_W \ \ln[P(W) \prod_l P(Y^l|X^l, W)]$$

$$\boxed{w_i \leftarrow w_i - \eta\lambda w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1|X^l, W))}$$

called a "<u>regularization</u>" term
• helps reduce overfitting, especially when training data is sparse
• keep weights nearer to zero (if P(W) is zero mean Gaussian prior), or whatever the prior suggests
• used very frequently in Logistic Regression

The Bottom Line

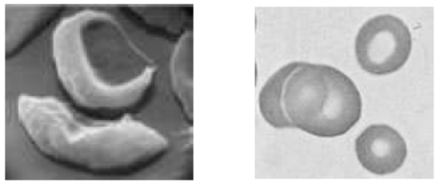
- Consider learning f: X →Y, where
  - X is a vector of real-valued features,$<X_1 \ldots X_n>$
  - Y is boolean
  - assume all X_i are conditionally independent given Y
  - model $P(X_i \mid Y = y_k)$ as Gaussian $N(\mu_{ik},\sigma_i)$
  - model P(Y) as Bernoulli (π)

- Then P(Y|X) is of this form, and we can directly estimate W

$$P(Y = 1|X =< X_1, ...X_n >) = \frac{1}{1 + exp(w_0 + \sum_i w_i X_i)}$$

- Furthermore, same holds if the X_i are boolean
  - trying proving that to yourself

Classification Tasks

	Features, X		Labels, Y
Diagnosing sickle cell anemia		⇨	Anemic cell Healthy cell
Tax Fraud Detection	<table><tr><th>Refund</th><th>Marital Status</th><th>Taxable Income</th></tr><tr><td>No</td><td>Married</td><td>80K</td></tr></table>	⇨	Cheat ?
Web Classification		⇨	Sports Science News
Predict squirrel hill resident	Drive to CMU, Rachel's fan, Shop at SH Giant Eagle	⇨	Resident Not resident

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Classification

Goal: Construct a **predictor** $f : X \to Y$ to minimize a risk (performance measure) $R(f)$

Sports
Science
News

Features, X

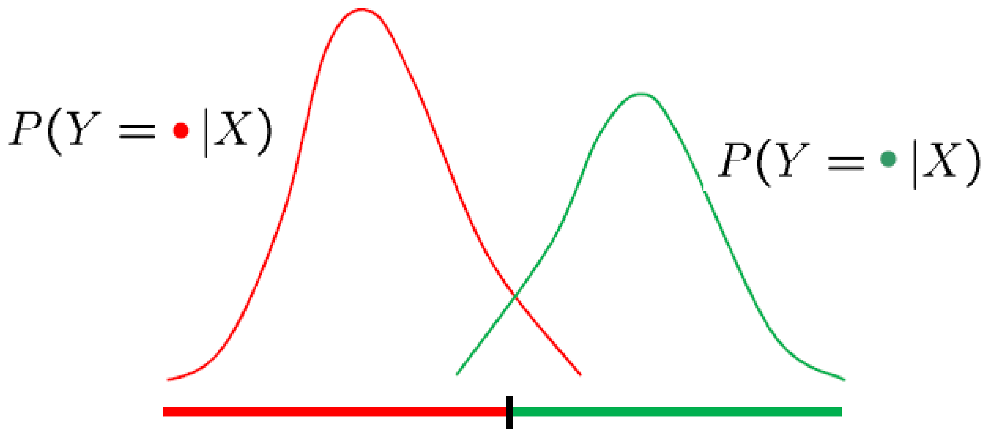
Labels, Y

$$R(f) = P(f(X) \neq Y)$$ **Probability of Error**

Classification

Optimal predictor:
(Bayes classifier)

$$f^* = \arg\min_f P(f(X) \neq Y)$$



$$f^*(X) = \begin{cases} \bullet & P(Y = \bullet|X) > P(Y = \bullet|X) \\ \bullet & \text{otherwise} \end{cases}$$

Depends on **unknown** distribution P_{XY}

Classification algorithms

However, we can **learn** a good prediction rule from **training data**

$$\{(X_i, Y_i)\}_{i=1}^{n} \overset{\text{iid}}{\sim} P_{XY}\,(\text{unknown})$$

Independent and identically distributed

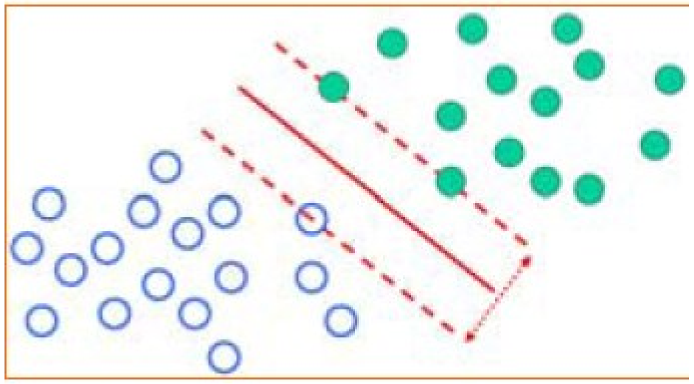
$$\begin{tikzcd}
\text{Training data} \quad \{(X_i, Y_i)\}_{i=1}^{n} \arrow[r] & \boxed{\textbf{Learning algorithm}} \arrow[r] & \text{Prediction rule} \quad \widehat{f}_n
\end{tikzcd}$$

So far ...

Decision Trees
K-Nearest Neighbor
Naïve Bayes
Logistic Regression

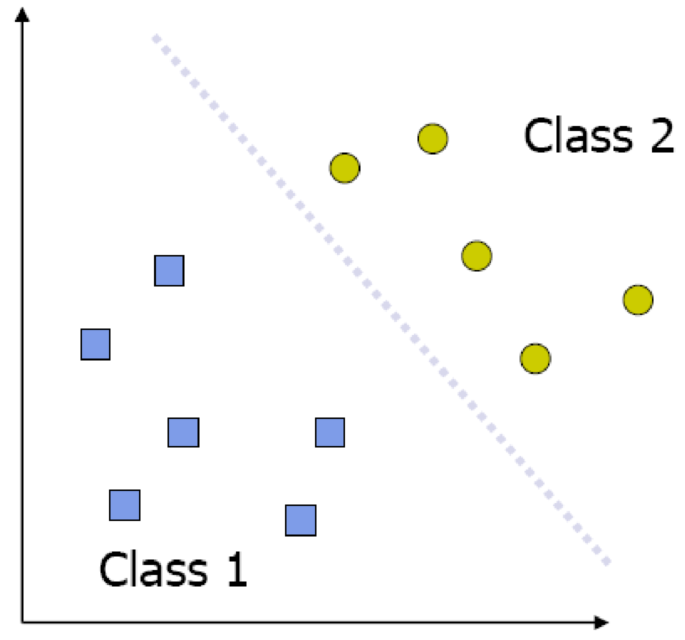
Machine Learning

Support Vector Machines

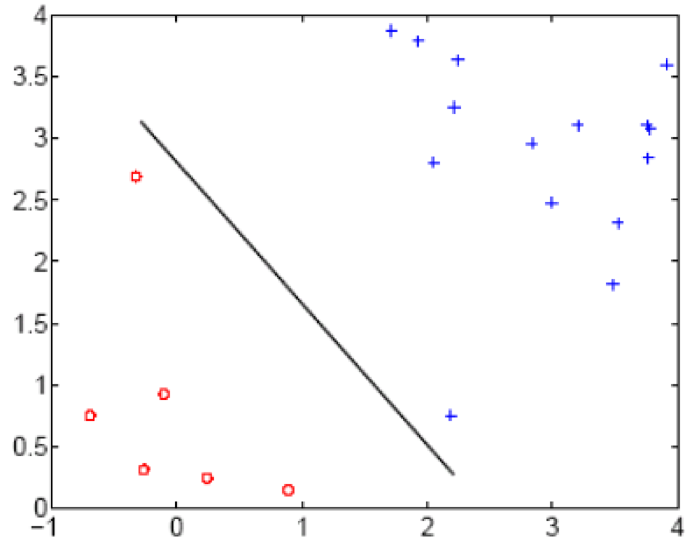


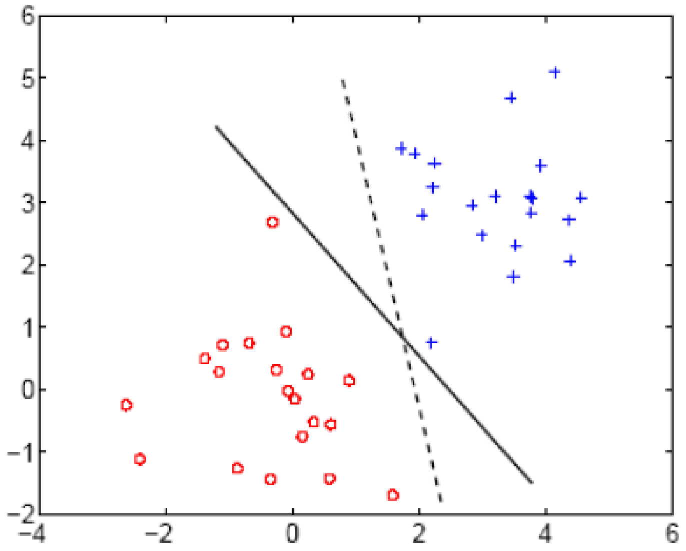
What is a good Decision Boundary?

- Consider a binary classification task with y = ±1 labels (not 0/1 as before).
- When the training examples are linearly separable, we can set the parameters of a linear classifier so that all the training examples are classified correctly
- Many decision boundaries!
  - Generative classifiers
  - Logistic regressions …
- Are all decision boundaries equally good?



Not All Decision Boundaries Are Equal!



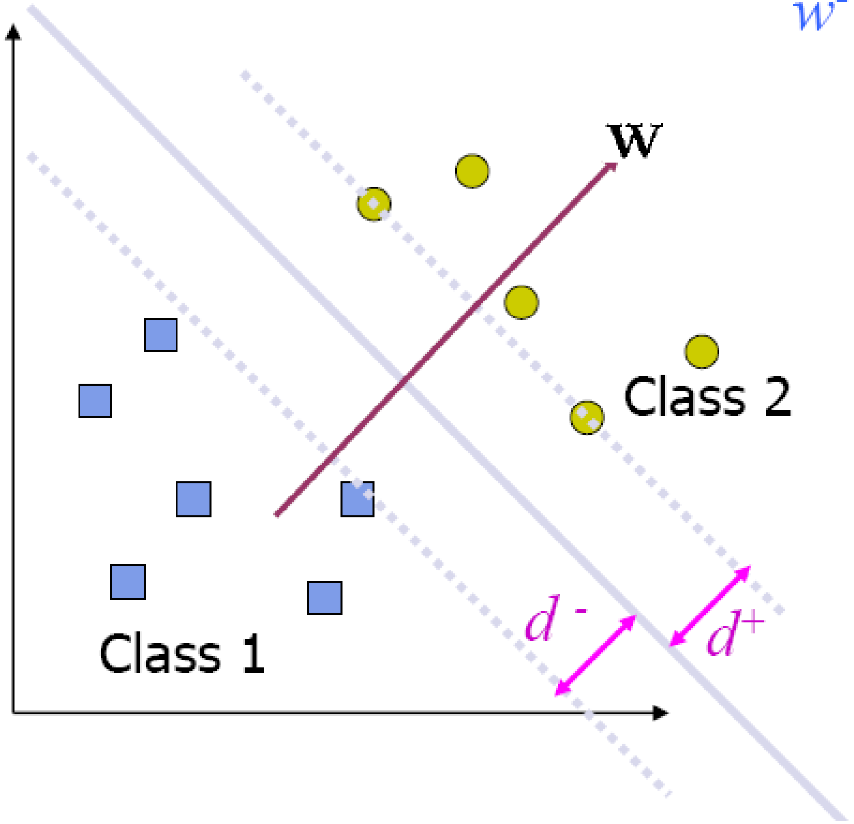


- **Why we may have such boundaries?**
  - **Irregular distribution**
  - **Imbalanced training sizes**
  - **outliners**

Classification and Margin

- Parameterzing decision boundary
  - Let ***w*** denote a vector orthogonal to the decision boundary, and ***b*** denote a scalar "offset" term, then we can write the decision boundary as:

$$w^T x + b = 0$$



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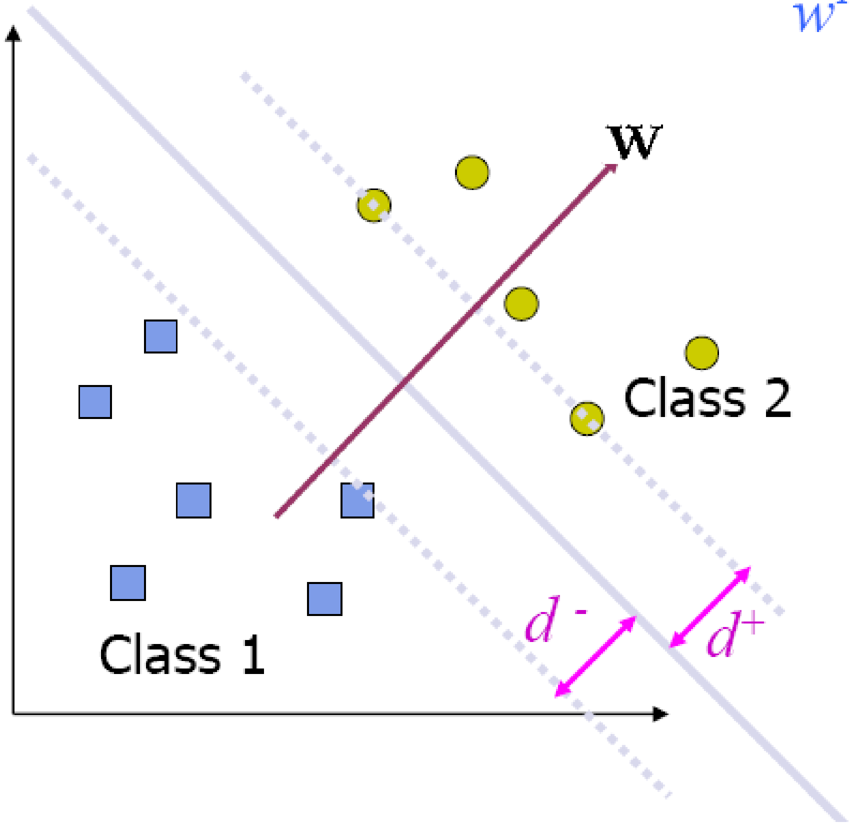


- Margin

$$w^T x_i + b > +c \qquad \text{for all } x_i \text{ in class 2}$$

$$w^T x_i + b < -c \qquad \text{for all } x_i \text{ in class 1}$$

Or more compactly:

$$(w^T x_i + b) y_i > c$$

The margin between any two points

$$\boldsymbol{m} = d^- + d^+ =$$

Maximum Margin Classification

- The "minimum" permissible margin is:

$$m = \frac{w^T}{\|w\|}\left(x_{i^*} - x_{j^*}\right) = \frac{2c}{\|w\|}$$

- Here is our Maximum Margin Classification problem:

$$\begin{array}{ll} \max_w & \dfrac{2c}{\|w\|} \\ \text{s.t} & y_i(w^T x_i + b) \geq c, \ \ \forall i \end{array}$$

Maximum Margin Classification, con'd.

- The optimization problem:

$$\max_{w,b} \quad \frac{c}{\|w\|}$$
$$\text{s.t} \quad y_i(w^T x_i + b) \geq c, \quad \forall i$$

- But note that the magnitude of c merely scales w and b, and does not change the classification boundary at all! (why?)
- So we instead work on this cleaner problem:

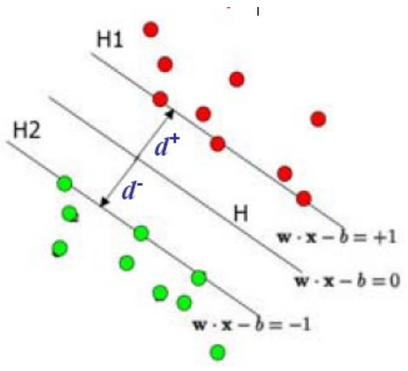
$$\max_{w,b} \quad \frac{1}{\|w\|}$$
$$\text{s.t} \quad y_i(w^T x_i + b) \geq 1, \quad \forall i$$

- The solution to this leads to the famous ***Support Vector Machines*** --- believed by many to be the best "off-the-shelf" supervised learning algorithm

Support vector machine

- A convex quadratic programming problem with linear constrains:

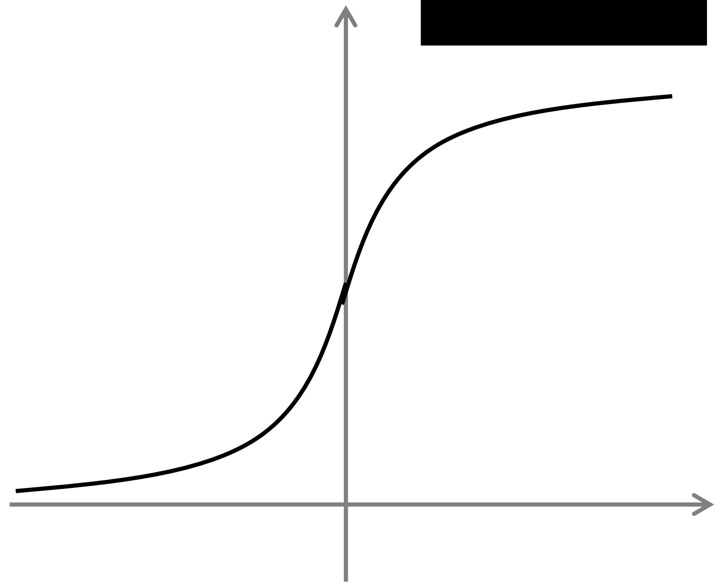
$$\max_{w,b} \quad \frac{1}{\|w\|}$$
$$\text{s.t} \quad y_i(w^T x_i + b) \geq 1, \quad \forall i$$


H1
H2
H
d^+
d^-
$\mathbf{w} \cdot \mathbf{x} - b = +1$
$\mathbf{w} \cdot \mathbf{x} - b = 0$
$\mathbf{w} \cdot \mathbf{x} - b = -1$

  - The attained margin is now given by $\frac{1}{\|w\|}$
  - Only a few of the classification constraints are relevant → **support vectors**
- Constrained optimization
  - We can directly solve this using commercial quadratic programming (QP) code
  - But we want to take a more careful investigation of Lagrange duality, and the solution of the above in its dual form.
    - deeper insight: support vectors, kernels …
    - more efficient algorithm

Alternative view of logistic regression

[redacted]



If [redacted] , we want [redacted] , [redacted]

If [redacted] , we want [redacted] , [redacted]

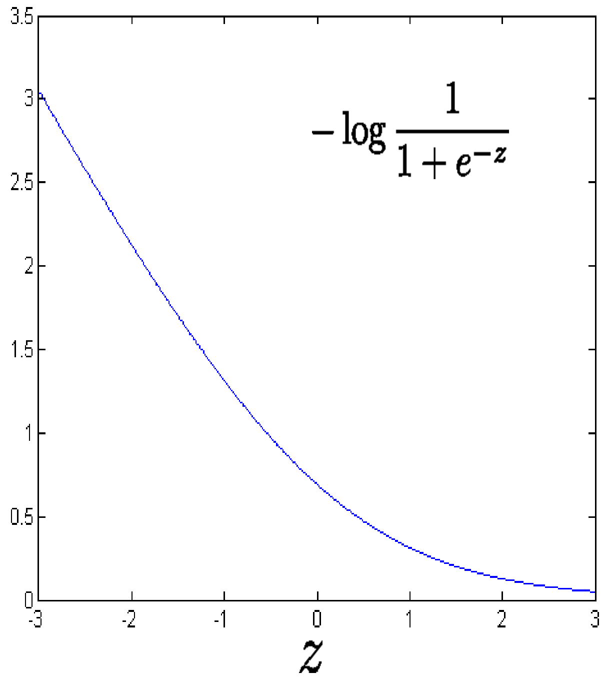
Alternative view of logistic regression

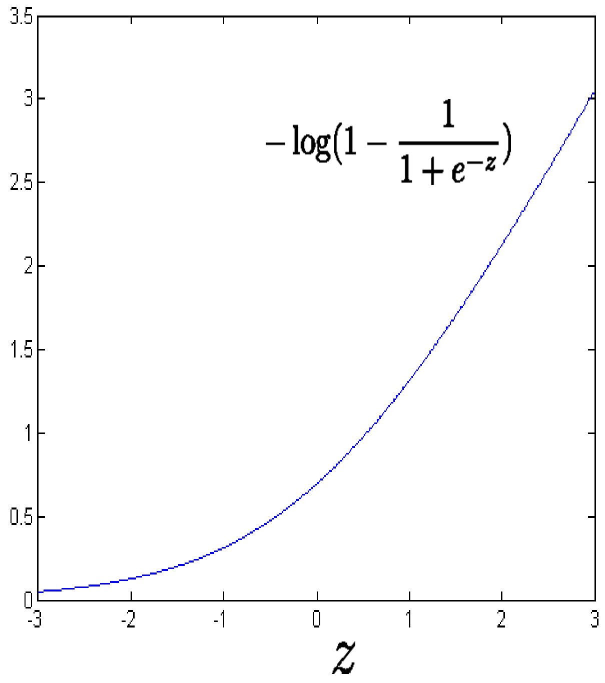
Cost of example: [redacted]

[redacted]

If $y = 1$ (want [redacted]):

If $y = 0$ (want [redacted]):





Support vector machine

Logistic regression:

$$\min_\theta \frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)}\left(-\log h_\theta(x^{(i)})\right) + (1-y^{(i)})\left((-\log(1-h_\theta(x^{(i)}))\right)\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

Support vector machine:

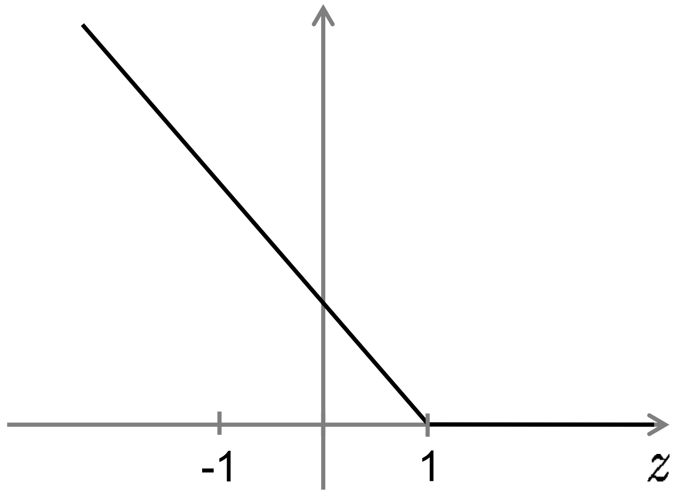
[redacted]

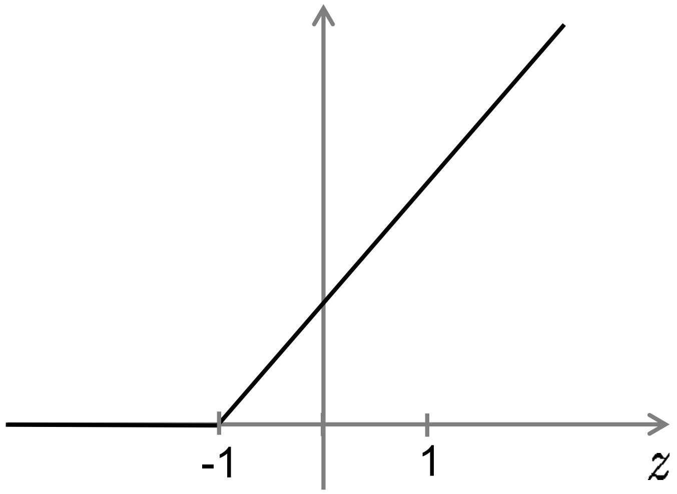
SVM hypothesis

Hypothesis:

Support Vector Machine

[redacted]





If [redacted] , we want [redacted] (not just [redacted])

If [redacted] , we want [redacted] (not just [redacted])

SVM Decision Boundary

[redacted]

Whenever [redacted] :

Whenever [redacted] :

Digression to Lagrangian Duality

- The Primal Problem

Primal:

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & g_i(w) \le 0, \quad i = 1, \dots, k \\ & h_i(w) = 0, \quad i = 1, \dots, l \end{aligned}$$

The generalized Lagrangian:

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

the α's ($\alpha_i \ge 0$) and βs are called the Lagarangian multipliers

Lemma:

$$\max_{\alpha, \beta, \alpha_i \ge 0} \mathcal{L}(w, \alpha, \beta) = \begin{cases} f(w) & \text{if } w \text{ satisfies primal constraints} \\ \infty & \text{o/w} \end{cases}$$

A re-written Primal:

$$\min_w \max_{\alpha, \beta, \alpha_i \ge 0} \mathcal{L}(w, \alpha, \beta)$$

Lagrangian Duality, cont.

- Recall the Primal Problem:

$$\min_w \max_{\alpha,\beta,\alpha_i\geq 0} \mathcal{L}(w,\alpha,\beta)$$

- The Dual Problem:

$$\max_{\alpha,\beta,\alpha_i\geq 0} \min_w \mathcal{L}(w,\alpha,\beta)$$

- **Theorem (weak duality):**

$$d^* = \max_{\alpha,\beta,\alpha_i\geq 0} \min_w \mathcal{L}(w,\alpha,\beta) \ \leq\ \min_w \max_{\alpha,\beta,\alpha_i\geq 0} \mathcal{L}(w,\alpha,\beta) = p^*$$

- **Theorem (strong duality):**

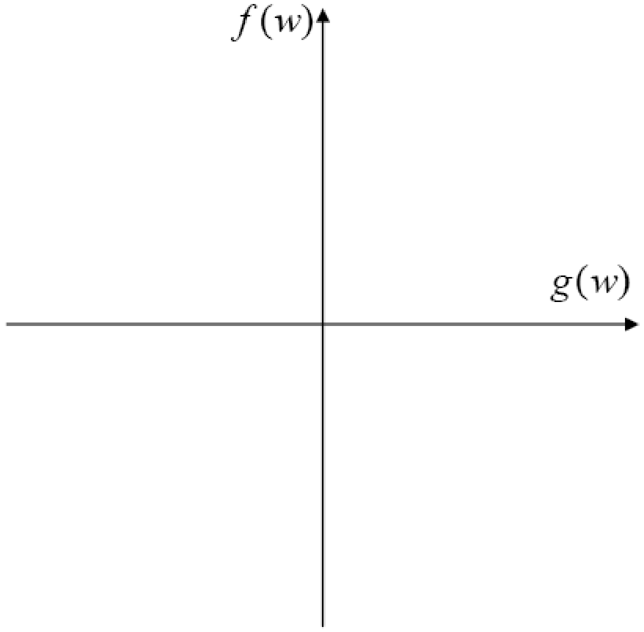
Iff there exist a saddle point of $\mathcal{L}(w,\alpha,\beta)$, we have

$$d^* = p^*$$

A sketch of strong and weak duality

- Now, ignoring *h*(*x*) for simplicity, let's look at what's happening graphically in the duality theorems.

$$d^* = \max_{\alpha_i \geq 0} \min_w f(w) + \alpha^T g(w) \;\leq\; \min_w \max_{\alpha_i \geq 0} f(w) + \alpha^T g(w) = p^*$$



The KKT conditions

- If there exists some saddle point of $\mathcal{L}$, then the saddle point satisfies the following "Karush-Kuhn-Tucker" (KKT) conditions:

$$\frac{\partial}{\partial w_i}\mathcal{L}(w,\alpha,\beta)=0, \quad i=1,\ldots,k$$

$$\frac{\partial}{\partial \beta_i}\mathcal{L}(w,\alpha,\beta)=0, \quad i=1,\ldots,l$$

$$\alpha_i g_i(w)=0, \quad i=1,\ldots,m$$ Complementary slackness

$$g_i(w)\le 0, \quad i=1,\ldots,m$$ Primal feasibility

$$\alpha_i \ge 0, \quad i=1,\ldots,m$$ Dual feasibility

- **Theorem**: If w^*, α^* and β^* satisfy the KKT condition, then it is also a solution to the primal and the dual problems.

Solving optimal margin classifier

- Recall our opt problem:

$$\begin{aligned} &\max_{w,b} \quad \frac{1}{\|w\|} \\ &\text{s.t} \quad y_i(w^T x_i + b) \geq 1, \quad \forall i \end{aligned}$$

- This is equivalent to

$$\begin{aligned} &\min_{w,b} \quad \frac{1}{2} w^T w \\ &\text{s.t} \quad 1 - y_i(w^T x_i + b) \leq 0, \quad \forall i \end{aligned} \qquad (*)$$

- Write the Lagrangian:

$$\mathcal{L}(w,b,\alpha) = \frac{1}{2} w^T w - \sum_{i=1}^{m} \alpha_i \left[y_i (w^T x_i + b) - 1 \right]$$

  - Recall that (*) can be reformulated as $\min_{w,b} \max_{\alpha_i \geq 0} \mathcal{L}(w,b,\alpha)$
    Now we solve its **dual problem**: $\max_{\alpha_i \geq 0} \min_{w,b} \mathcal{L}(w,b,\alpha)$

The Dual Problem

$$\max_{\alpha_i \geq 0} \min_{w,b} \mathcal{L}(w,b,\alpha)$$

- We minimize $\mathcal{L}$ with respect to w and b first:

$$\nabla_w \mathcal{L}(w,b,\alpha) = w - \sum_{i=1}^{m} \alpha_i y_i x_i = 0, \qquad (*)$$

$$\nabla_b \mathcal{L}(w,b,\alpha) = \sum_{i=1}^{m} \alpha_i y_i = 0, \qquad (**)$$

Note that (*) implies:

$$w = \sum_{i=1}^{m} \alpha_i y_i x_i \qquad (***)$$

- Plus (***) back to $\mathcal{L}$, and using (**), we have:

$$\mathcal{L}(w,b,\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

The Dual problem, cont.

- Now we have the following dual opt problem:

$$\max_{\alpha} \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

$$\text{s.t.} \quad \alpha_i \geq 0, \quad i = 1, \ldots, k$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0.$$

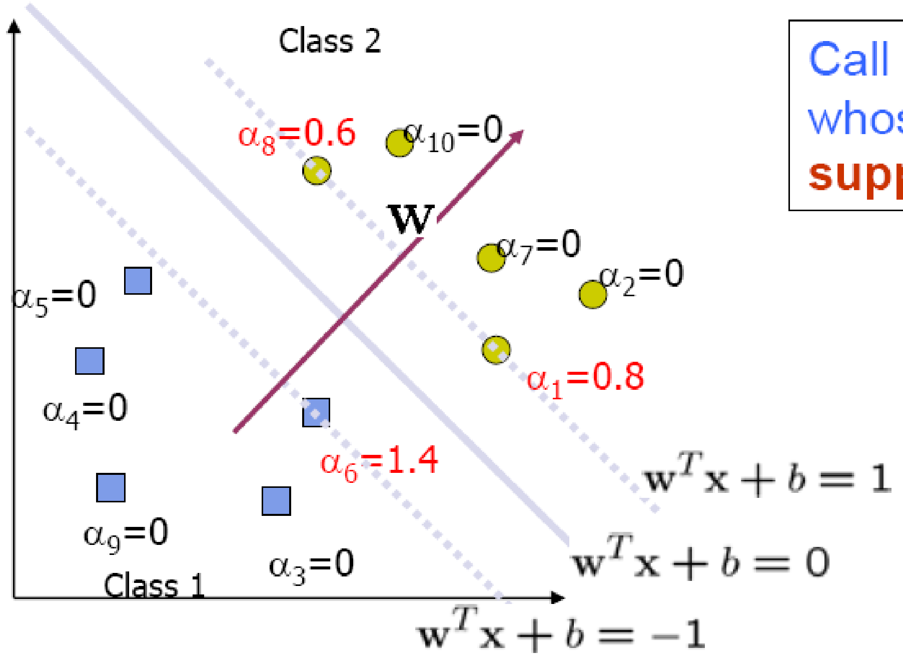
- This is, (again,) a **quadratic programming** problem.
  - A global maximum of α_i can always be found.
  - But what's the big deal??
  - Note two things:

1. w can be recovered by $w = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$ See next …
2. The "kernel" $\mathbf{x}_i^T \mathbf{x}_j$ More later …

Support vectors

- Note the KKT condition --- only a few α_i's can be nonzero!!

$$\alpha_i g_i(w) = 0, \quad i = 1, \ldots, m$$



Call the training data points whose α_i's are nonzero the **support vectors** (SV)

Support vector machines

- Once we have the Lagrange multipliers $\{\alpha_i\}$, we can reconstruct the parameter vector w as a weighted combination of the training examples:

$$w = \sum_{i \in SV} \alpha_i y_i \mathbf{x}_i$$

- For testing with a new data z
  - Compute

$$w^T z + b = \sum_{i \in SV} \alpha_i y_i \left(\mathbf{x}_i^T z \right) + b$$

  and classify z as class 1 if the sum is positive, and class 2 otherwise
  - Note: w need not be formed explicitly

Interpretation of support vector machines

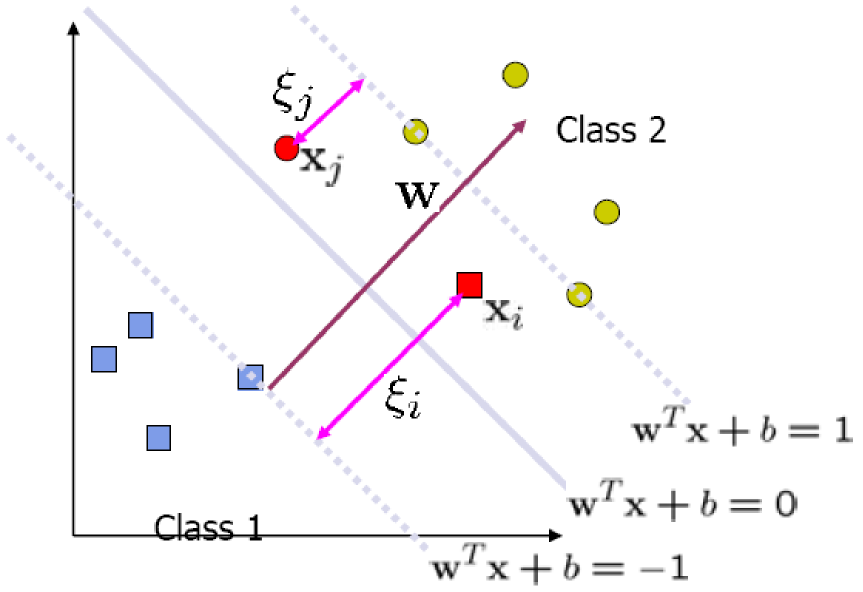
- The optimal w is a linear combination of a small number of data points. This “sparse” representation can be viewed as data compression as in the construction of kNN classifier

- To compute the weights $\{\alpha_i\}$, and to use support vector machines we need to specify only the inner products (or kernel) between the examples $\mathbf{x}_i^T \mathbf{x}_j$

- We make decisions by comparing each new example z with only the support vectors:

$$y^* = \operatorname{sign}\left(\sum_{i \in SV} \alpha_i y_i \left(\mathbf{x}_i^T z \right) + b \right)$$

Non-linearly Separable Problems



ξ_j
$\mathbf{x}_j$
$\mathbf{w}$
Class 2
$\mathbf{x}_i$
ξ_i
$\mathbf{w}^T\mathbf{x}+b=1$
$\mathbf{w}^T\mathbf{x}+b=0$
Class 1
$\mathbf{w}^T\mathbf{x}+b=-1$

- We allow "error" ξ_i in classification; it is based on the output of the discriminant function $\boldsymbol{w}^T\boldsymbol{x}+b$
- ξ_i approximates the number of misclassified samples

Soft Margin Hyperplane

- Now we have a slightly different opt problem:

$$\min_{w,b} \quad \frac{1}{2} w^T w + C \sum_{i=1}^{m} \xi_i$$

$$\text{s.t} \quad \begin{aligned} & y_i(w^T x_i + b) \geq 1 - \xi_i, \quad \forall i \\ & \xi_i \geq 0, \quad \forall i \end{aligned}$$

  - ξ_i are "slack variables" in optimization
  - Note that ξ_i=0 if there is no error for $\mathbf{x}_i$
  - ξ_i is an upper bound of the number of errors
  - *C* : tradeoff parameter between error and margin

The Optimization Problem

- The dual of this new constrained optimization problem is

$$\max_{\alpha} \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

$$\text{s.t.} \quad 0 \leq \alpha_i \leq C, \quad i = 1, \ldots, m$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0.$$

- This is very similar to the optimization problem in the linear separable case, except that there is an upper bound *C* on α_i now
- Once again, a QP solver can be used to find α_i

Non-linear Decision Boundary

- So far, we have only considered large-margin classifier with a linear decision boundary
- How to generalize it to become nonlinear?
- Key idea: transform $\mathbf{x}_i$ to a higher dimensional space to "make life easier"
  - Input space: the space the point xi are located
  - Feature space: the space of φ(xi) after transformation

- Why transform?
  - Linear operation in the feature space is equivalent to non-linear operation in input space
  - Classification can become easier with a proper transformation. In the XOR problem, for example, adding a new feature of x_1x_2 make the problem linearly separable

The XOR problem

A classic problem is the `XOR` problem. The training data for this is:

$$\left\{\left\{\begin{bmatrix}1.0\\-1.0\end{bmatrix},1\right\},\left\{\begin{bmatrix}-1.0\\1.0\end{bmatrix},1\right\},\left\{\begin{bmatrix}1.0\\1.0\end{bmatrix},-1\right\},\left\{\begin{bmatrix}-1.0\\-1.0\end{bmatrix},-1\right\}\right\}$$

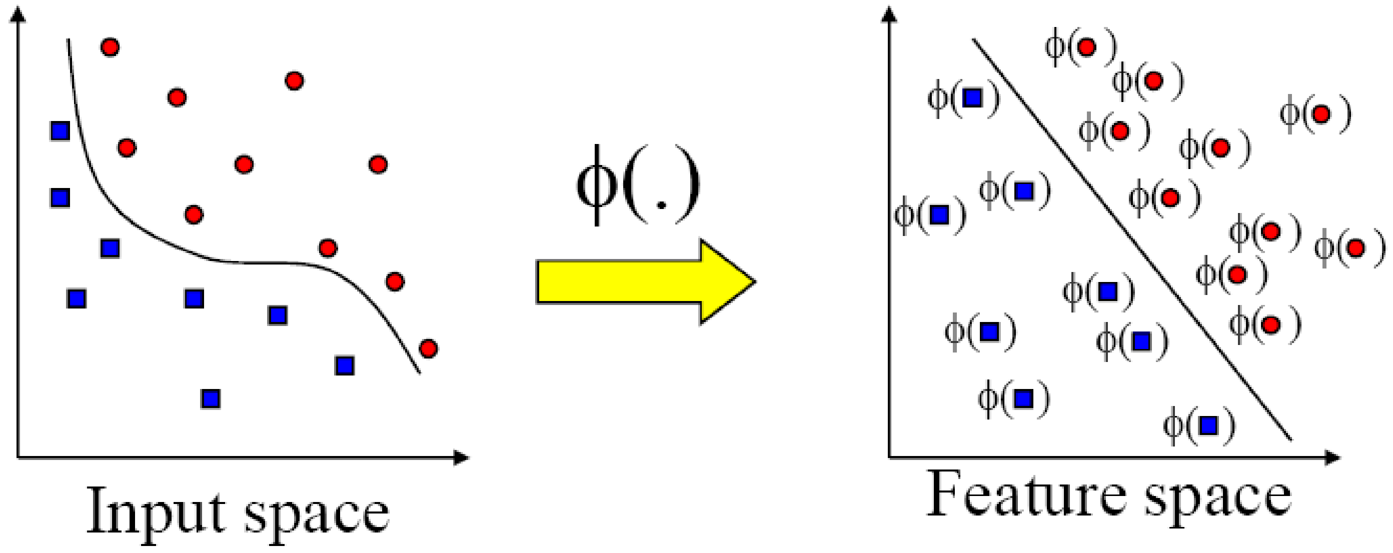
This data is clearly not separable with a linear decision boundary. Consider the following mapping:

$$\boldsymbol{x} = \begin{bmatrix}x_1\\x_2\end{bmatrix} \rightarrow \boldsymbol{\Phi}(\boldsymbol{x}) = \begin{bmatrix}1\\\sqrt{2}x_1\\\sqrt{2}x_2\\\sqrt{2}x_1x_2\\x_1^2\\x_2^2\end{bmatrix}$$

Each point is now mapped from a 2-dimensional space to a 5-dimensional space. The data is separable in this high dimensional space.

Non-linear Decision Boundary

Transforming the Data



Note: feature space is of higher dimension than the input space in practice

The Kernel Trick

- Recall the SVM optimization problem

$$\max_{\alpha} \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

$$\text{s.t.} \quad 0 \le \alpha_i \le C, \quad i = 1, \ldots, m$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0.$$

- The data points only appear as inner product
- As long as we can calculate the inner product in the feature space, we do not need the mapping explicitly
- Many common geometric operations (angles, distances) can be expressed by inner products
- Define the kernel function *K* by $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$

An Example for feature mapping and kernels

- Consider an input $\mathbf{x}=[x_1,x_2]$
- Suppose $\phi(.)$ is given as follows

$$\phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = 1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2$$

- An inner product in the feature space is

$$\left\langle \phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right), \phi\left(\begin{bmatrix} x_1' \\ x_2' \end{bmatrix}\right) \right\rangle =$$

- So, if we define the **kernel function** as follows, there is no need to carry out $\phi(.)$ explicitly

$$K(\mathbf{x},\mathbf{x}') = \left(1 + \mathbf{x}^T\mathbf{x}'\right)^2$$

More examples of kernel functions

- Linear kernel (we've seen it)

$$K(\mathbf{x},\mathbf{x}')=\mathbf{x}^T\mathbf{x}'$$

- Polynomial kernel (we just saw an example)

$$K(\mathbf{x},\mathbf{x}')=\left(1+\mathbf{x}^T\mathbf{x}'\right)^p$$

where p = 2, 3, … To get the feature vectors we concatenate all pth order polynomial terms of the components of x (weighted appropriately)

- Radial basis kernel

$$K(\mathbf{x},\mathbf{x}')=\exp\left(-\frac{1}{2}\left\|\mathbf{x}-\mathbf{x}'\right\|^2\right)$$

In this case the feature space consists of functions and results in a non-parametric classifier.

The essence of kernel

- Feature mapping, but "without paying a cost"
  - E.g., polynomial kernel

$$K(x,z) = (x^T z + c)^d$$

  - How many dimensions we've got in the new space?
  - How many operations it takes to compute K()?

- Kernel design, any principle?
  - K(x,z) can be thought of as a similarity function between x and z
  - This intuition can be well reflected in the following "Gaussian" function

    (Similarly one can easily come up with other K() in the same spirit)

$$K(x,z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right)$$

  - Is this necessarily lead to a "legal" kernel?

    (in the above particular case, K() is a legal one, do you know how many dimension ϕ(x) is?