CSDS 440: Machine Learning

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Office hours T, Th 11:15-11:45 or by appointment

Announcements

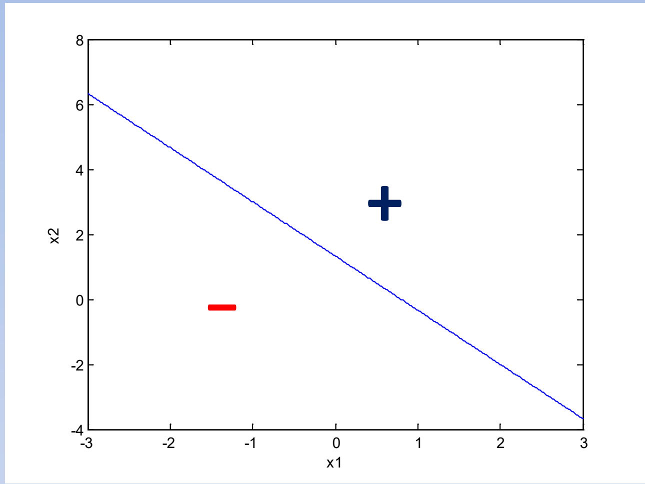
- Project due date changed to 12/8 11:59pm

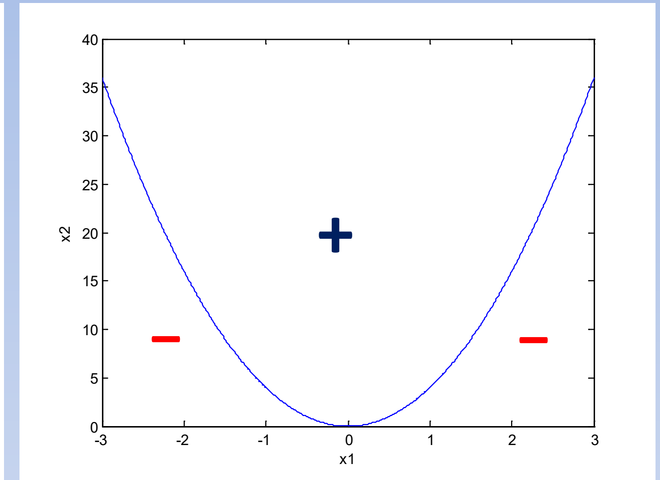
Support Vector Machines

- Combines three fundamental ideas
  - Linear discriminants
  - Margins
  - Kernels

- A theoretically well justified and empirically well-behaved method arising from three fields: ML (Cortes & Vapnik), Statistics (Wahba), Operations Research (Mangasarian)

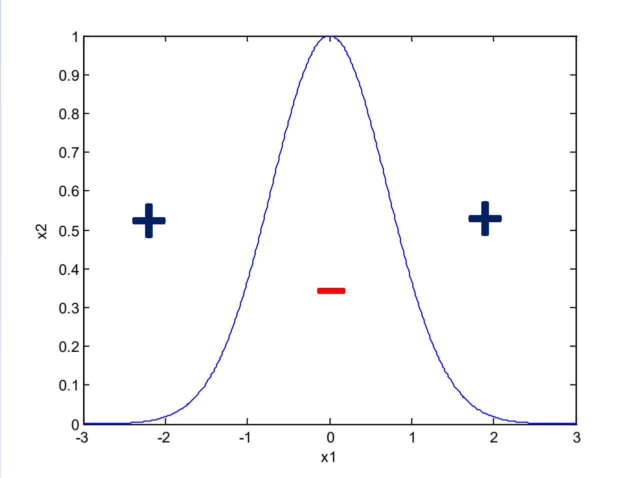
What is a “linear discriminant”?





$$sign(5x_1 + 3x_2 - 4)$$

$$sign(x_2 - 4x_1^2)$$



$$sign(x_2 - e^{-x_1^2})$$

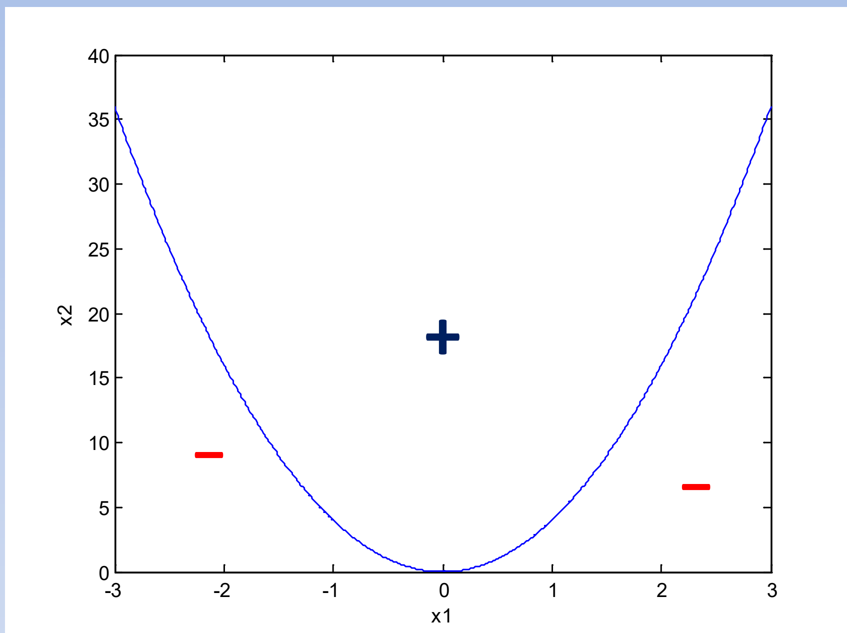
Linear Discriminants

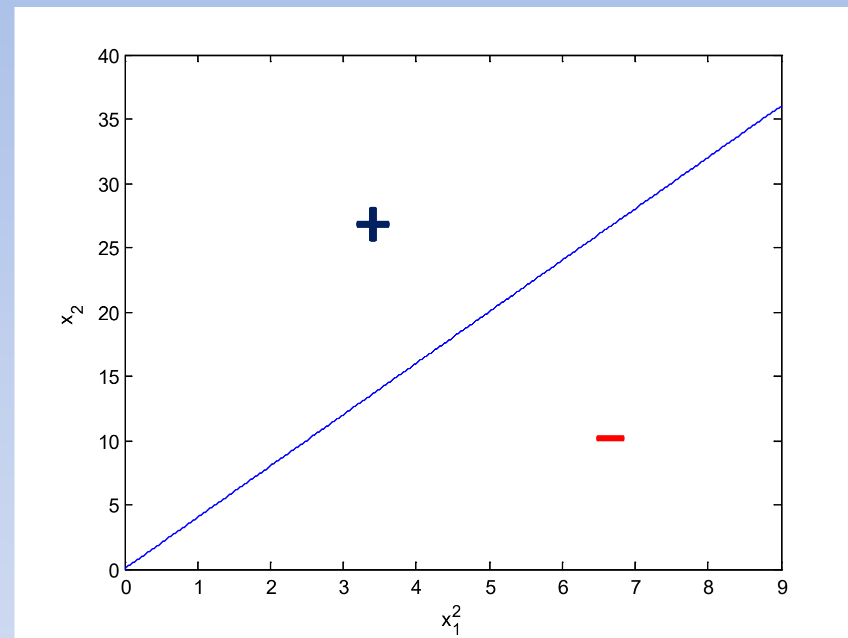
- We generally take "linear" to mean linear in the classifier parameters
  - Linear in $\mathbf{w}$, but not necessarily in $\mathbf{x}$
- A linear discriminant has the general form

$$\mathbf{w} \bullet \varphi(\mathbf{x}) + b = 0$$

- Here $\boldsymbol{\varphi}$ ("feature map") is any vector function from the domain of $\mathbf{x}$ to R^m
  - $\mathbf{x}$ need not be a number
  - φ could be arbitrary-dimensional

Linear Discriminants





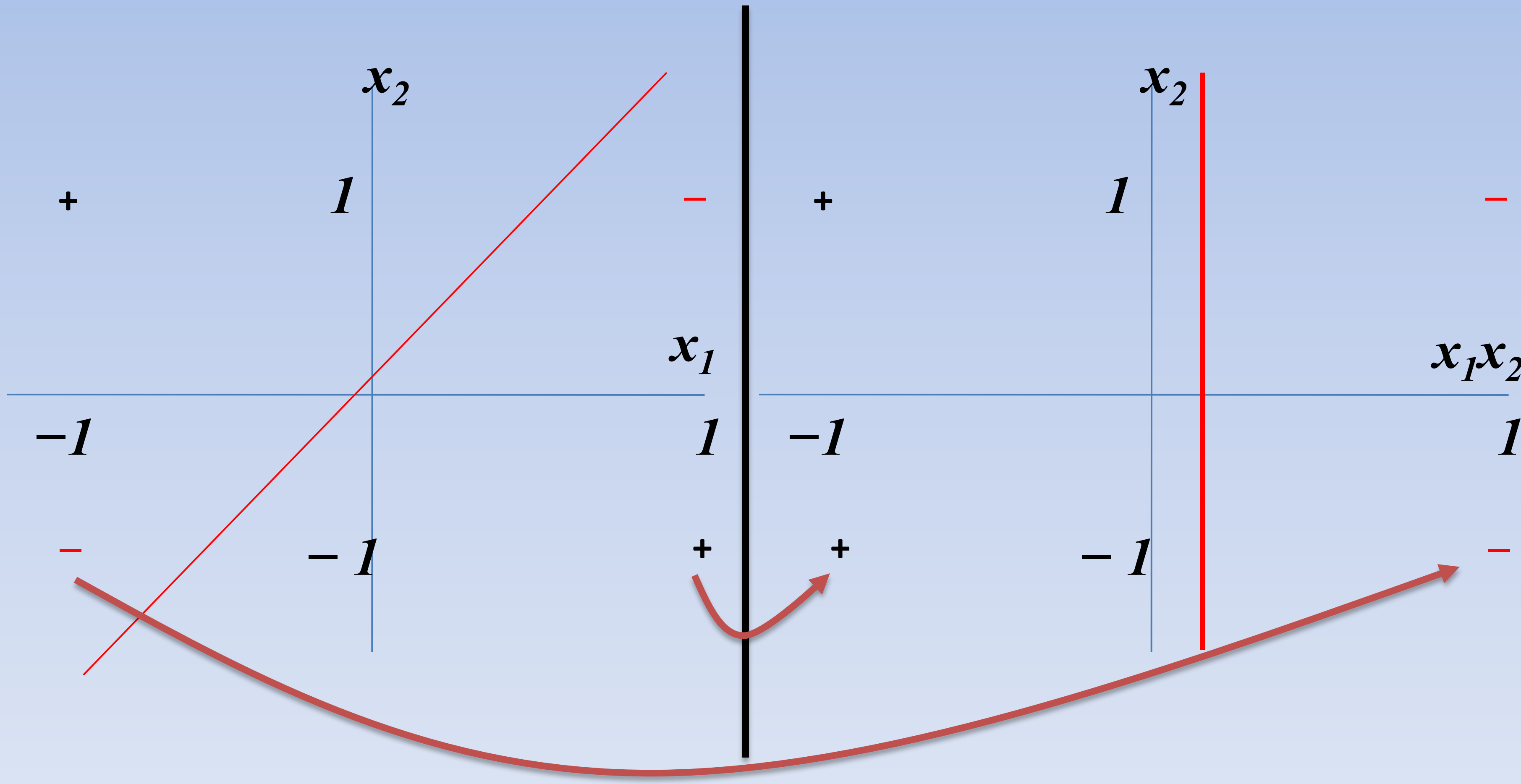
$$sign(x_2 - 4x_1^2)$$

$$\varphi(\mathbf{x}) = (x_1^2, x_2)$$

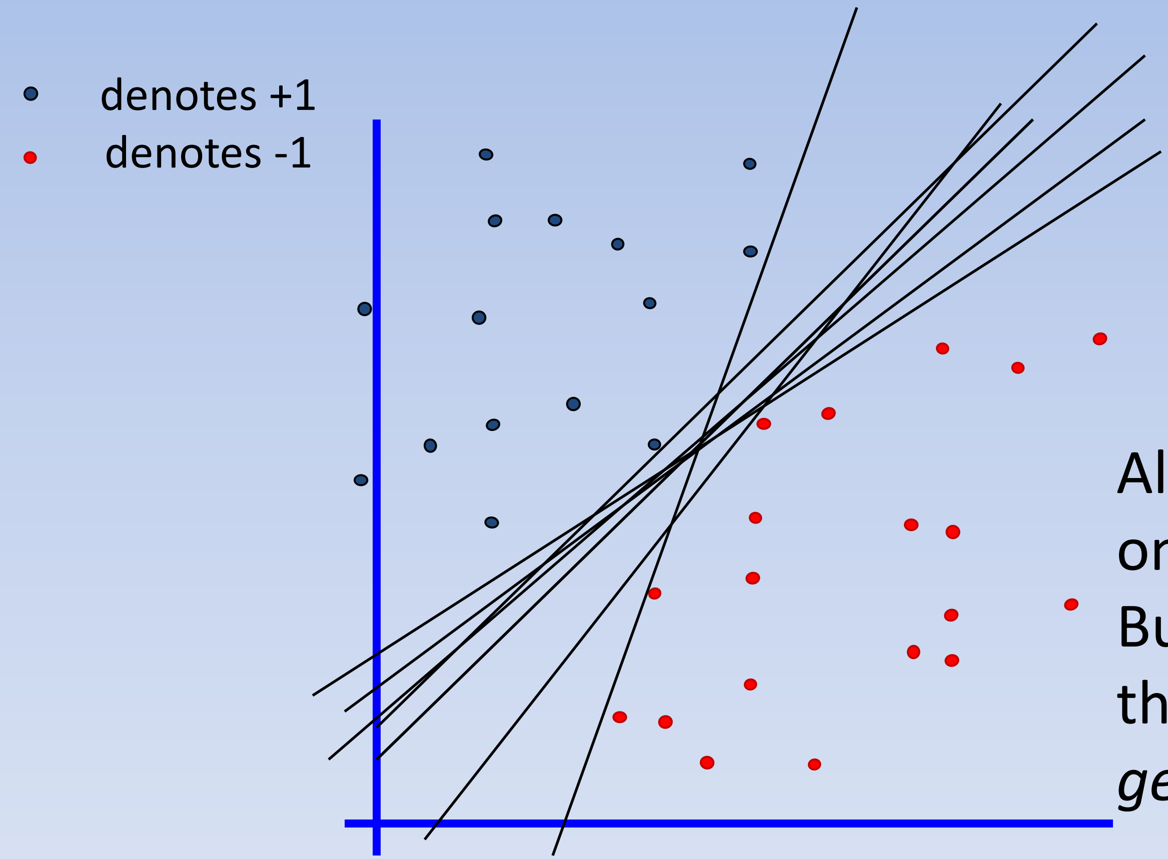
$$sign(\varphi_2(\mathbf{x}) - 4\varphi_1(\mathbf{x}))$$

φ maps features to an m-dimensional vector space

XOR and the Linear Discriminant



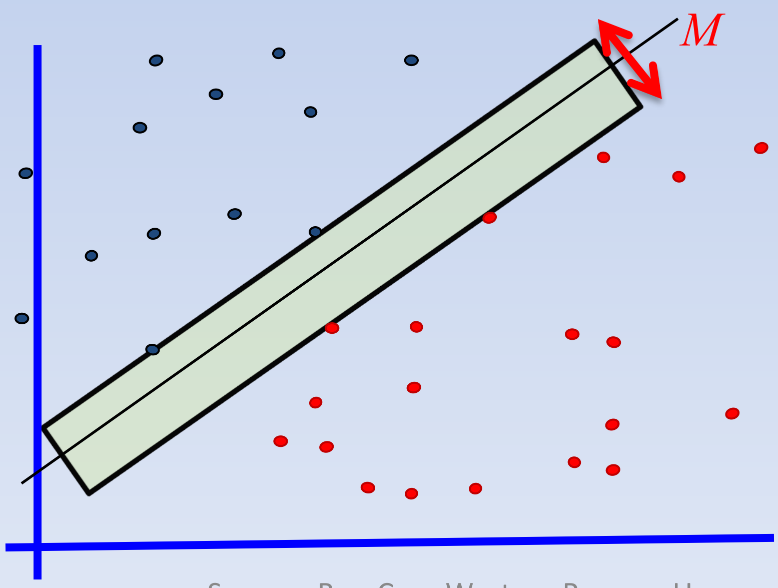
Find the Classifier



All are equally good on the training sample. But is there any one that we expect to *generalize* best?

Margin of a Classifier

- Imagine sliding any linear classifier parallel to itself
- The sum of the amounts we can move until we hit an (some) example(s) is the margin



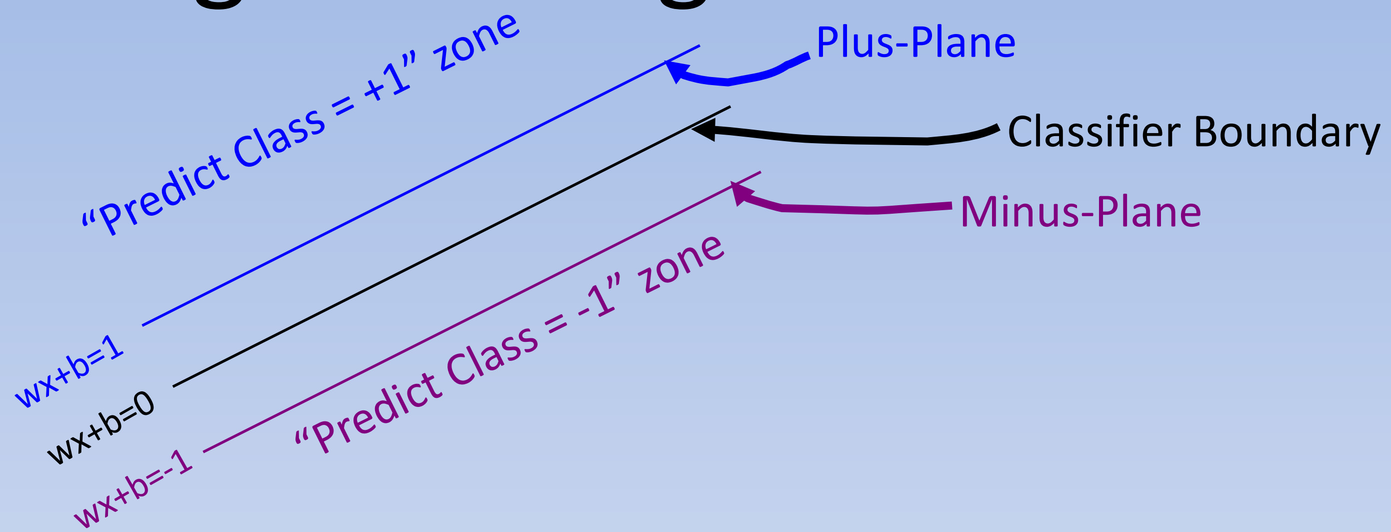
Support Vector Machine

- The linear classifier with the maximum margin is called a support vector machine classifier
- If we are in the input feature space , i.e. $\boldsymbol{\varphi}(\mathbf{x})=\mathbf{x}$, this is called a linear SVM
- The examples that touch the margin boundaries are called the support vectors

Why does this make sense?

- Intuitively, “maximum margin” gives greatest robustness to errors in the data
  - Generalization error is inversely proportional to margin (Bartlett and Shawe-Taylor 1998)
- The classifier depends on only a few data points, so it is
  - “Sparse” (has few parameters to learn)
  - Efficient to evaluate

Calculating the Margin



- Plus-plane = $\mathbf{w}\cdot\mathbf{x} + b = +1$
- Minus-plane = $\mathbf{w}\cdot\mathbf{x} + b = -1$

Classify as.. $+1$ if $\mathbf{w}\cdot\mathbf{x} + b \geq 1$

-1 if $\mathbf{w}\cdot\mathbf{x} + b \leq -1$

Calculating the Margin

- First note that $\mathbf{w}$ is perpendicular to the plane $\mathbf{w}\cdot\mathbf{x}+b=0$
- Why?
  - Pick $\mathbf{u}$, $\mathbf{v}$ on plane
  - $\mathbf{w}\cdot(\mathbf{u}-\mathbf{v})=\mathbf{w}\cdot\mathbf{u} - \mathbf{w}\cdot\mathbf{v}=(-b) -(- b)=0$
- So $\mathbf{w}$ is also perpendicular to the plus and minus planes

Calculating the Margin

- Choose an arbitrary point $\mathbf{x}^+$ on the plus plane and its nearest point $\mathbf{x}^-$ on the minus plane
- Notice that $\mathbf{x}^+ - \mathbf{x}^- = \lambda\mathbf{w}$ and so $M = \|\lambda\mathbf{w}\|_2$

$$\mathbf{w}\bullet\mathbf{x}^+ + b = 1$$

$$\mathbf{w}\bullet(\mathbf{x}^- + \lambda\mathbf{w}) + b = 1$$

$$\lambda\mathbf{w}\bullet\mathbf{w} = 2; \lambda = \frac{2}{\mathbf{w}\bullet\mathbf{w}} = \frac{2}{\|\mathbf{w}\|^2}$$

$$M = \|\lambda\mathbf{w}\| = \frac{2}{\|\mathbf{w}\|}$$

So maximizing the margin is equivalent here to minimizing the norm of the parameter vector! Also a rationale behind other overfitting control methods like weight decay

Problem Formulation

- On the training set,
  - Maximize the margin
  - *While respecting the labels of the training examples*
- Maximize the margin

$$\max_{\mathbf{w},b} \frac{2}{\|\mathbf{w}\|} = \min_{\mathbf{w},b} \frac{\|\mathbf{w}\|^2}{2}$$

Problem Formulation

- While respecting the labels of training examples---these are *constraints*

$$
\begin{aligned}
&\mathbf{w}\bullet\mathbf{x}_i + b \geq 1 \text{ if } y_i = 1\\
&\mathbf{w}\bullet\mathbf{x}_i + b \leq -1 \text{ if } y_i = -1\\
&\Rightarrow\\
&y_i(\mathbf{w}\bullet\mathbf{x}_i + b) \geq 1
\end{aligned}
$$

One such constraint for each example

Problem Formulation

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{so that } \forall i, y_i(\mathbf{w} \bullet \mathbf{x}_i + b) \geq 1$$

- Called a "quadratic program"
  - Many methods to solve, e.g. successive linearization
- Has globally unique solution! (convexity)
- So are we done?

Problem Formulation

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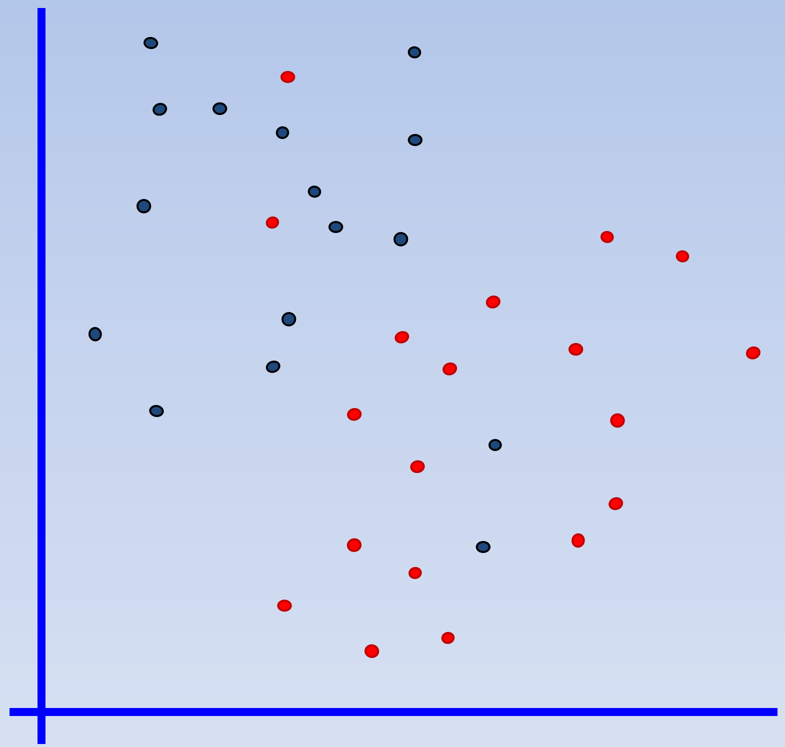
Linearly Inseparable Data



What happens to the QP in this case?

Linearly Inseparable Data

- Normally, we have:

$$y_i(\mathbf{w} \bullet \mathbf{x}_i + b) \geq 1$$

- So to allow for a misclassified point:

$$y_i(\mathbf{w} \bullet \mathbf{x}_i + b) \leq 1$$

$$\text{or } y_i(\mathbf{w} \bullet \mathbf{x}_i + b) + \xi_i \geq 1,\ \xi_i \geq 0$$

Free "slack" variables. The optimizer will find these values as well.

Problem Formulation, LI Data

$$\min_{\mathbf{w},b,\xi_i} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{so that } \forall i, y_i(\mathbf{w}\bullet\mathbf{x}_i + b) + \xi_i \geq 1, \xi_i \geq 0$$

Oops, doesn't work!! Try $\mathbf{w}$=0, b=0, ξ_i=1. Can't just allow for misclassified points---must *minimize the number of misclassified points as well*!

LI Data, Attempt 2

- Want:

$$\min_{\mathbf{w},b,\xi_i} \frac{1}{2}\left\|\mathbf{w}\right\|^2 + [Number\_of\_errors]$$

$$\text{so that } \forall i, y_i(\mathbf{w} \bullet \mathbf{x}_i + b) + \xi_i \geq 1, \xi_i \geq 0$$

- But this is problematic, because number of errors is not a differentiable quantity

LI Data, Attempt 2

- We know that:

$$y_i(\mathbf{w}\bullet\mathbf{x}_i + b) + \xi_i \geq 1, \xi_i \geq 0,$$

$$\text{So } \xi_i \geq 1 - y_i(\mathbf{w}\bullet\mathbf{x}_i + b)$$

- So $0 \leq \xi_i < 1$ for correctly classified points, and $\xi_i \geq 1$ for incorrectly classified points

- So $\sum \xi_i$ is an upper bound on the number of errors
  - This is a differentiable quantity we can minimize

Final Formulation

Tradeoff between generalization and error

Slack for i^{th} example

$$\min_{\mathbf{w},b,\xi_i} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \xi_i$$

$$\text{so that } \forall i, y_i(\mathbf{w}\bullet\mathbf{x}_i + b) + \xi_i \geq 1$$

$$\text{and} \qquad \forall i, \xi_i \geq 0$$

Nonlinear (in $\mathbf{x}$) Classifiers

- So far, we have looked at SVMs linear in $\mathbf{x}$

- How do we learn decision surfaces nonlinear in $\mathbf{x}$?

SVM Formulation

$$\min_{\mathbf{w},b,\xi_i} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \xi_i$$

$$\text{so that } \forall i, y_i(\mathbf{w}\bullet\varphi(\mathbf{x}_i)+b)+\xi_i \geq 1$$

$$\text{and} \qquad \forall i, \xi_i \geq 0$$

Nonlinear (in $\mathbf{x}$) Classifiers

- But it turns out we need not explicitly compute $\varphi(x)$ at all!
  - Using "kernels" (different from CNN kernels)
  - "Implicit feature map"
  - Computational savings

- To get this, we will build the *dual form* of the linear SVM's QP using the "Generalized Lagrangian"

Recall: Duality in Linear Programming

- From any "primal" LP, we can derive a "dual" LP in the following way:

$$\min_{\mathbf{x}} c^T \mathbf{x}$$
$$s.t.\quad A\mathbf{x} \geq b$$
$$\mathbf{x} \geq 0$$

"Primal" problem

$$\max_{\mathbf{u}} b^T \mathbf{u}$$
$$s.t.\quad A^T \mathbf{u} \leq c$$
$$\mathbf{u} \geq 0$$

"Dual" problem

Generalized Lagrangian

- Consider the following problem:

$$\min_w f(w)$$
$$\text{so that } g_i(w) \le 0$$
$$\text{and} \qquad h_j(w) = 0$$

- The generalized Lagrangian is defined by:

$$\ell(w, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(w) + \sum_i \alpha_i g_i(w) + \sum_j \beta_j h_j(w)$$

“Langrangian multipliers”

For the linearly-separable SVM

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{so that } \forall i, -\left[y_i(\mathbf{w}\bullet\mathbf{x}_i + b) - 1\right] \le 0$$

$$\therefore \ell(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_i \alpha_i \left[y_i(\mathbf{w}\bullet\mathbf{x}_i + b) - 1\right]$$

Lagrange Duality

- Consider $P(w) = \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\boldsymbol{\alpha}\geq 0} \ell(w, \boldsymbol{\alpha}, \boldsymbol{\beta})$

$$P(w) = \max_{\alpha,\beta:\alpha\geq 0} f(w) + \sum_i \alpha_i g_i(w) + \sum_j \beta_j h_j(w)$$

"Primal" problem

$$= \begin{cases} f(w) \text{ if constraints on } g \text{ and } h \text{ are met} \\ \infty \text{ else} \end{cases}$$

- So the original problem can be written as

$$\min_w P(w) = \min_w \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\boldsymbol{\alpha}\geq 0} \ell(w, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

Lagrange Duality

- Consider $\max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\boldsymbol{\alpha}\geq 0} D(\boldsymbol{\alpha},\boldsymbol{\beta}) = \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\boldsymbol{\alpha}\geq 0} \min_{w} \ell(w,\boldsymbol{\alpha},\boldsymbol{\beta})$
- This is the dual formulation corresponding to P
  - So starting with ℓ, we can *derive* the dual for a primal problem

For the linearly-separable SVM

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{so that } \forall i, -\left[y_i(\mathbf{w}\bullet\mathbf{x}_i + b) - 1\right] \leq 0$$

$$\therefore \ell(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_i \alpha_i \left[y_i(\mathbf{w}\bullet\mathbf{x}_i + b) - 1\right]$$

Linearly-separable SVM, Dual Form

$$\ell(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_i \alpha_i \left[y_i (\mathbf{w} \bullet \mathbf{x}_i + b) - 1 \right]$$

$$\nabla_{\mathbf{w}} \ell(\mathbf{w}, b, \boldsymbol{\alpha}) = \mathbf{w} - \sum_i \alpha_i y_i \mathbf{x}_i = 0$$

$$\therefore \mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

$$\nabla_b \ell(\mathbf{w}, b, \boldsymbol{\alpha}) = \sum_i \alpha_i y_i = 0$$

Substitute for $\mathbf{w}$ in ℓ

Linearly-separable SVM, Dual Form

$$\ell(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_i \alpha_i \left[y_i(\mathbf{w} \bullet \mathbf{x}_i + b) - 1 \right]$$

$$\mathbf{w} = \sum_j \alpha_j y_j \mathbf{x}_j ; \sum_i \alpha_i y_i = 0$$

Substitute for $\mathbf{w}$ in ℓ

$$D(\boldsymbol{\alpha}) = \frac{1}{2}\sum_{i,j} y_i y_j \alpha_i \alpha_j \mathbf{x}_i \bullet \mathbf{x}_j + \sum_i \alpha_i - \sum_{i,j} y_i y_j \alpha_i \alpha_j \mathbf{x}_i \bullet \mathbf{x}_j - b\sum_i \alpha_i y_i$$

$$= \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} y_i y_j \alpha_i \alpha_j \mathbf{x}_i \bullet \mathbf{x}_j$$

Linearly-separable SVM, Dual Form

$$\max_{\alpha} D(\boldsymbol{\alpha}) = \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} y_i y_j \alpha_i \alpha_j \mathbf{x}_i \bullet \mathbf{x}_j$$

$$\text{so that } \boldsymbol{\alpha} \geq 0, \sum_i \alpha_i y_i = 0$$

From derivative w.r.t b

Karush-Kuhn-Tucker conditions

- At the optimal primal/dual solution, the following conditions will hold:

$$\nabla_{\mathbf{w},b}\ell(\mathbf{w}^*, b^*, \boldsymbol{\alpha}^*) = 0$$

Gradient at solution is zero

$$-\left[y_i(\mathbf{w}^* \bullet \mathbf{x}_i + b^*) - 1 \right] \le 0$$

All constraints satisfied

$$\alpha_i^* \ge 0$$

$$\alpha_i^* \left[y_i(\mathbf{w}^* \bullet \mathbf{x}_i + b^*) - 1 \right] = 0$$

KKT dual complementarity
If i^{th} LM is positive, the i^{th} constraint is "active", i.e. zero
These are the **support vectors**

These conditions are **necessary and sufficient!**