Center for Data Science
NYU

DS-GA 3001.007
Introduction to Machine Learning

Lecture 11

Support Vector Machines and Kernels

Classifying with Margins through Hinge Loss function

DS-GA 3001.007 Introduction to Machine Learning

Replacing features with relationships between features

Lecture 11

Support Vector Machines and Kernels

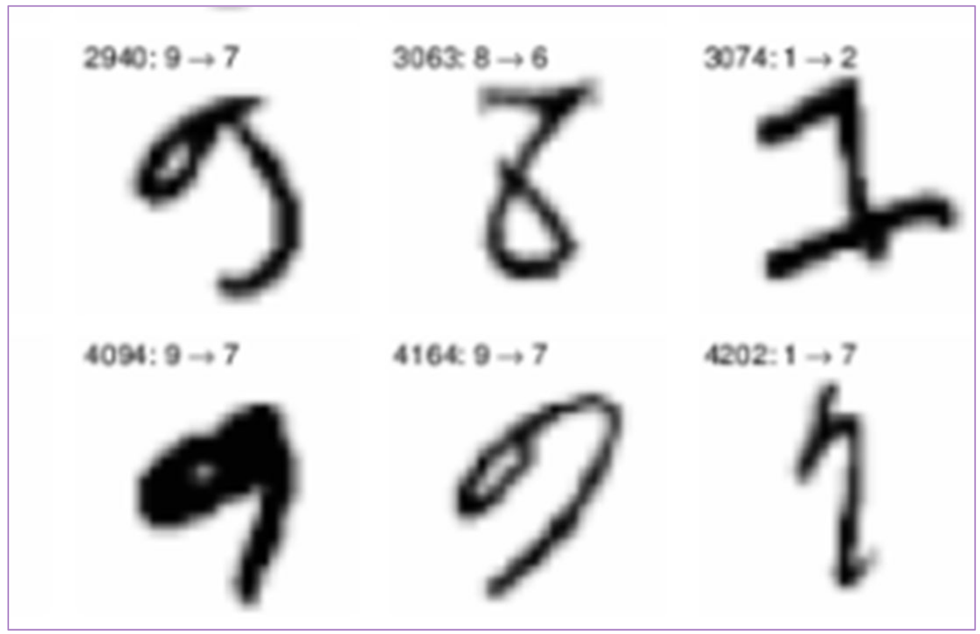
Announcements

- Homework
  - Homework 4 extended to **Wednesday November 13** at 11:59pm
  - Homework 5 due **Tuesday November 26** at 11:59pm
- Project
  - Milestone due **Thursday November 28** at 11:59pm
  - Background and Plans
- Labs
  - Submit on Jupyter Hub under Assignments tab

Refer to weekly agenda for more information

Homework 5

- Kernel Methods
  - New Kernels from Old Kernels
  - Modifying Pegasos Algorithm for Kernelized SVM
  - Image Classification
    - MNIST dataset of handwritten characters
    - 10 categories not 2 categories



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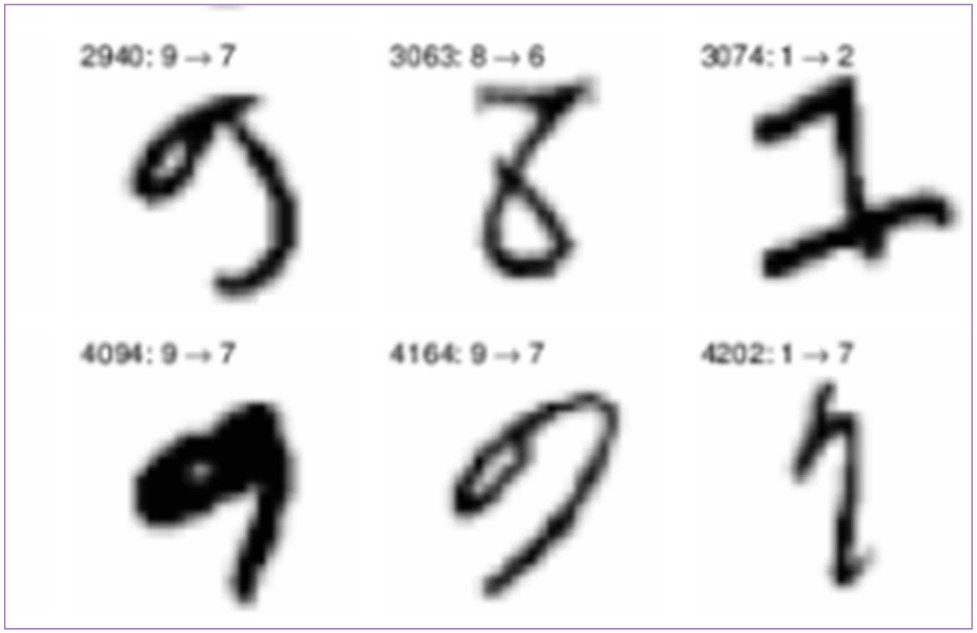
To check that kernel corresponds to relationship between features we would need to determine the feature transformation…



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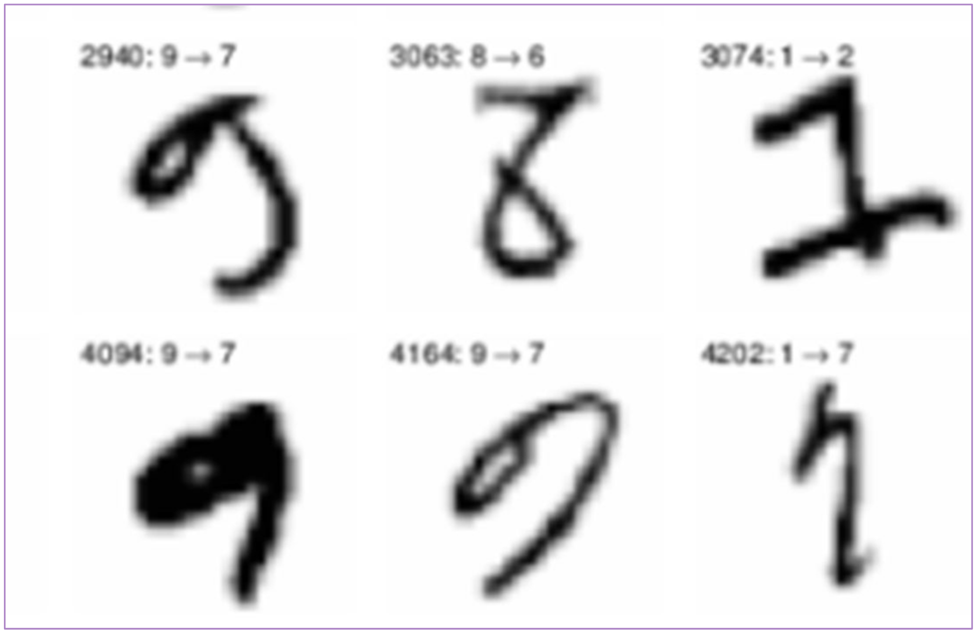
...instead express new kernel in terms of old kernel through scaling, sums and products



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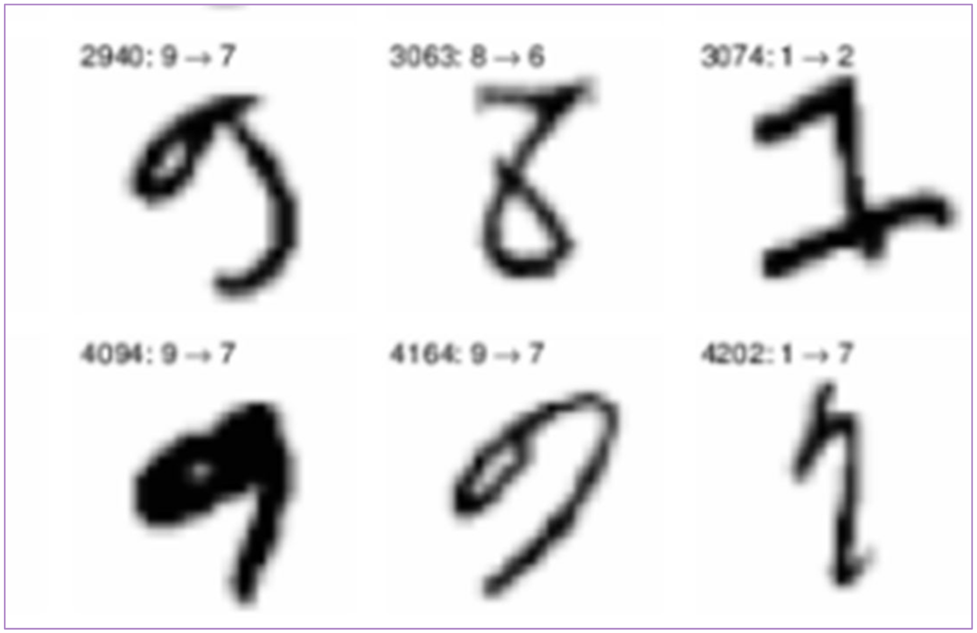
Pegasos is Stochastic Subgradient descent for Hinge Loss and L2 regularization with decreasing learning rate.



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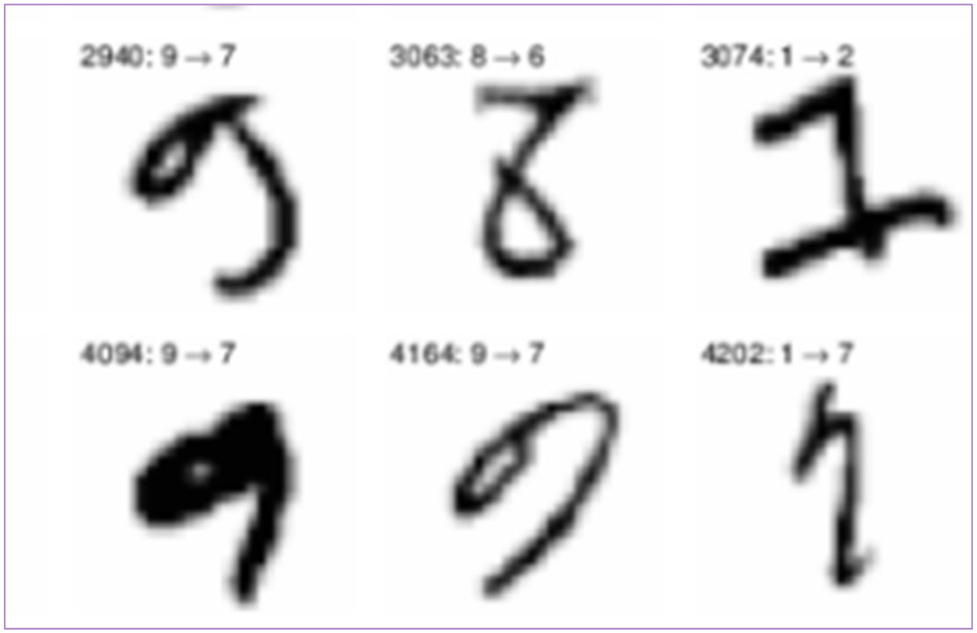
Kernelized SVM means expressing the weights in different way…



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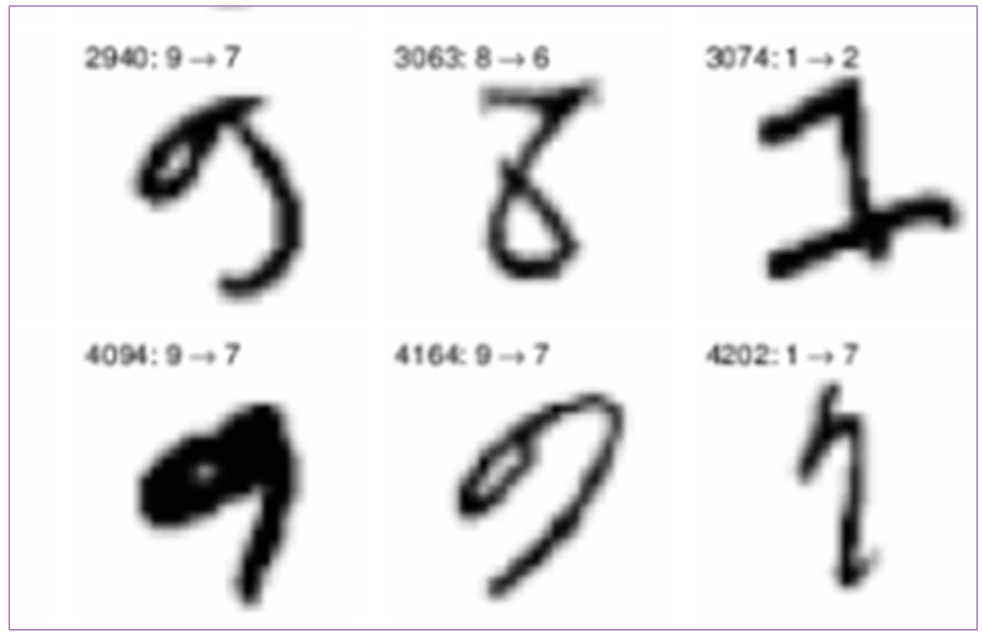
…you will determine the different update step in the algorithm to change your implementation



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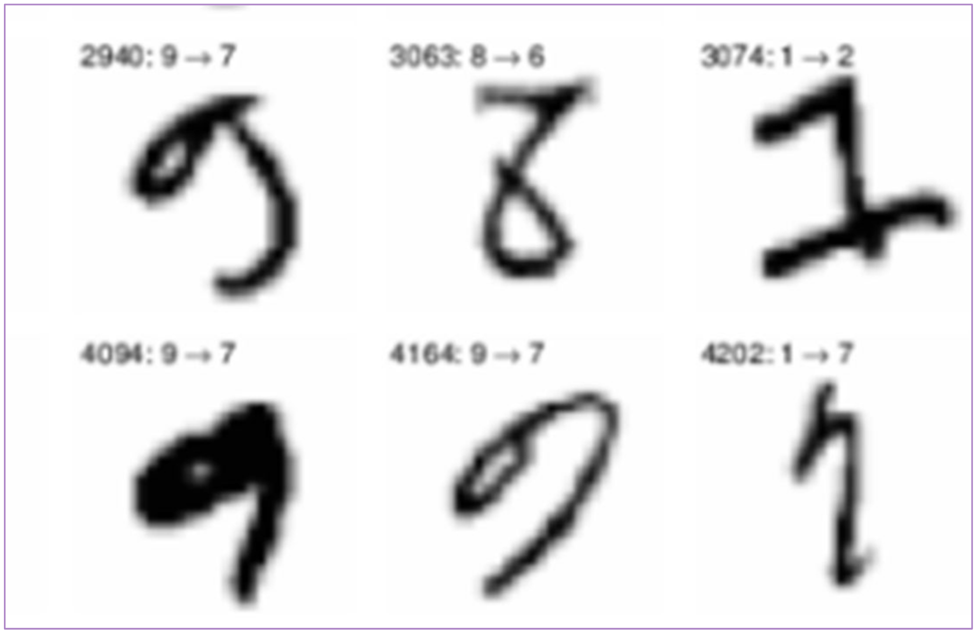

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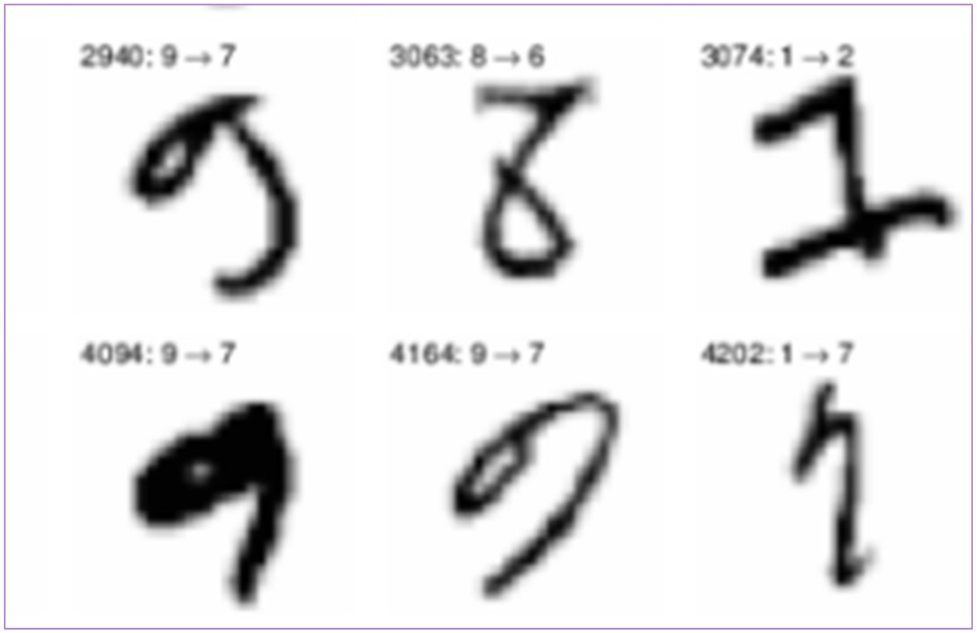
Training set 2000 handwritten digits. Test set 1000 handwritten digits. First column is label. Feature is 28x28 greyscale image.



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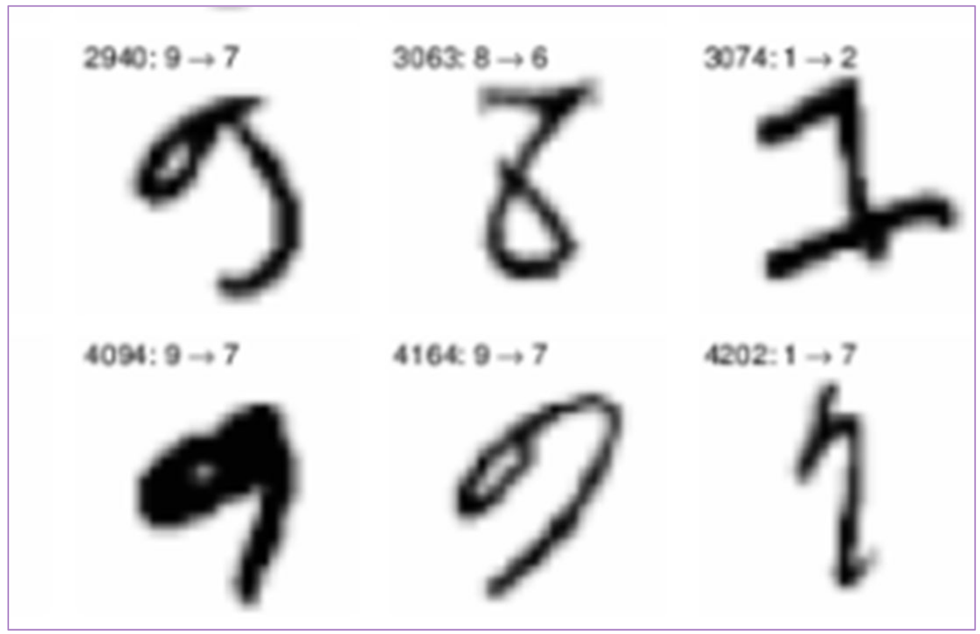
Classify into multiple categories…we will discuss one-vs-all classification next week



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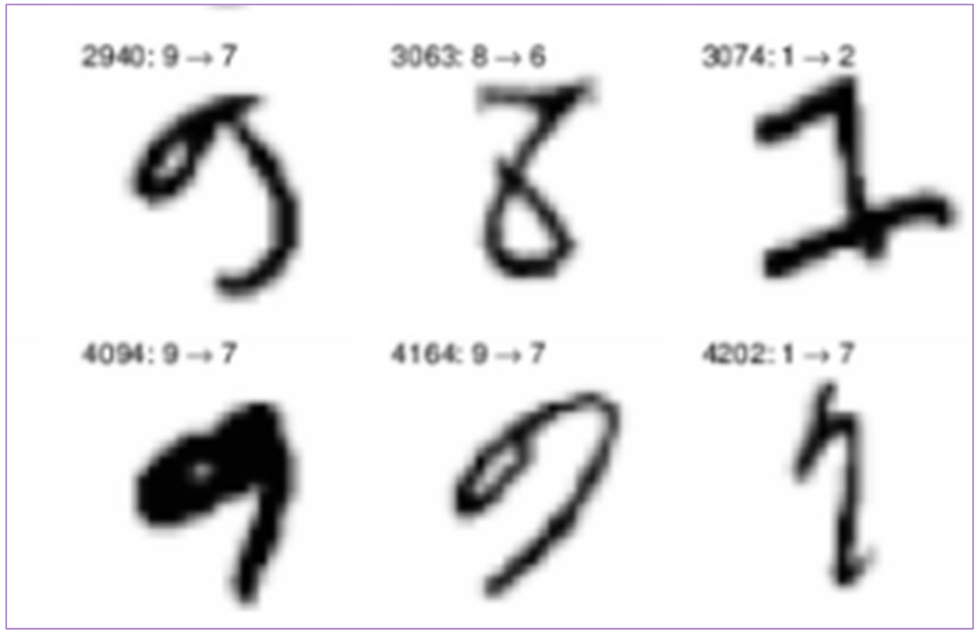
You will use your implementation of Pegasos and libSVM in sklearn that implements SMO…



…think of SMO as line search for quadratic programming problems because it changes variables two at a time.

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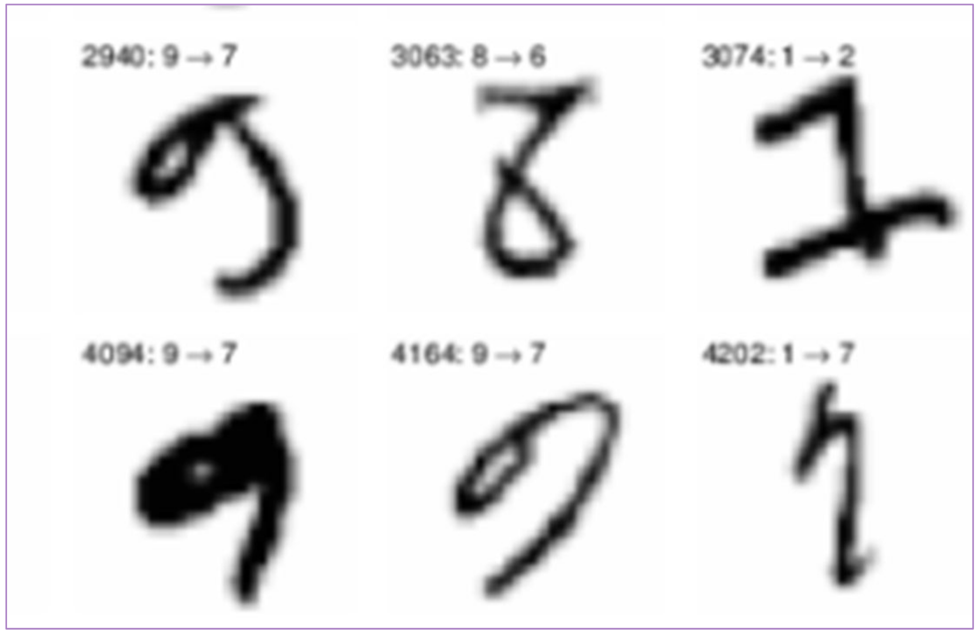

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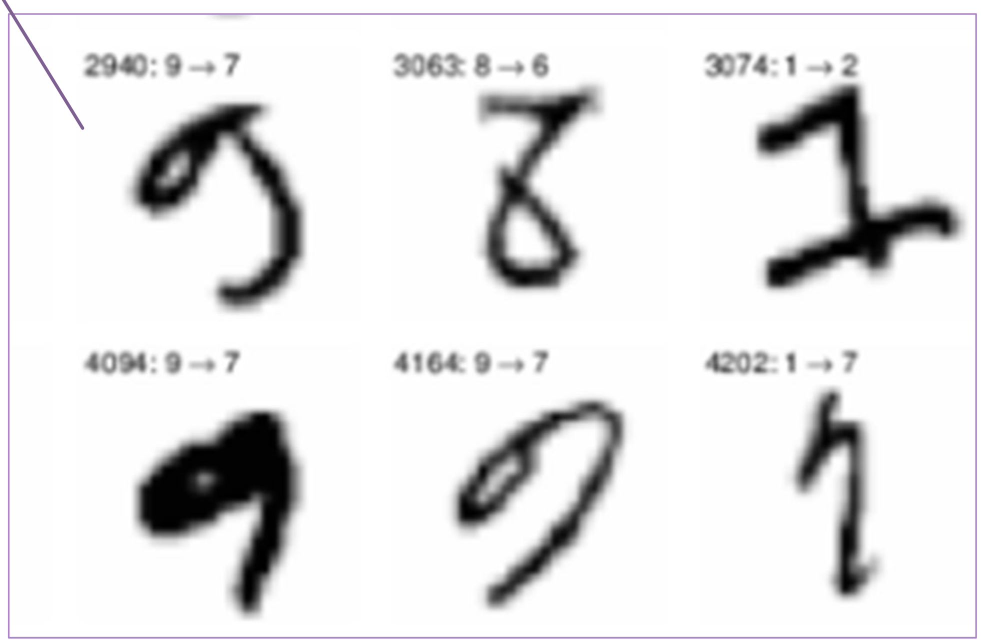
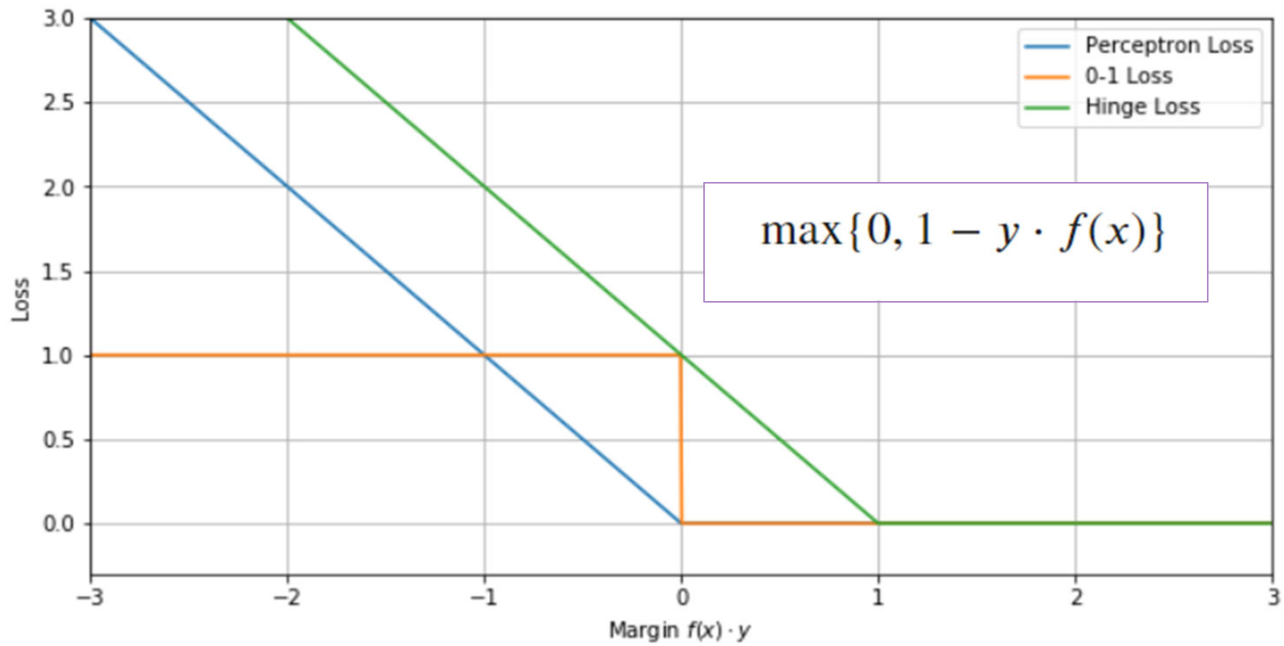
http://scs.ryerson.ca/~aharley/vis/conv/flat.html



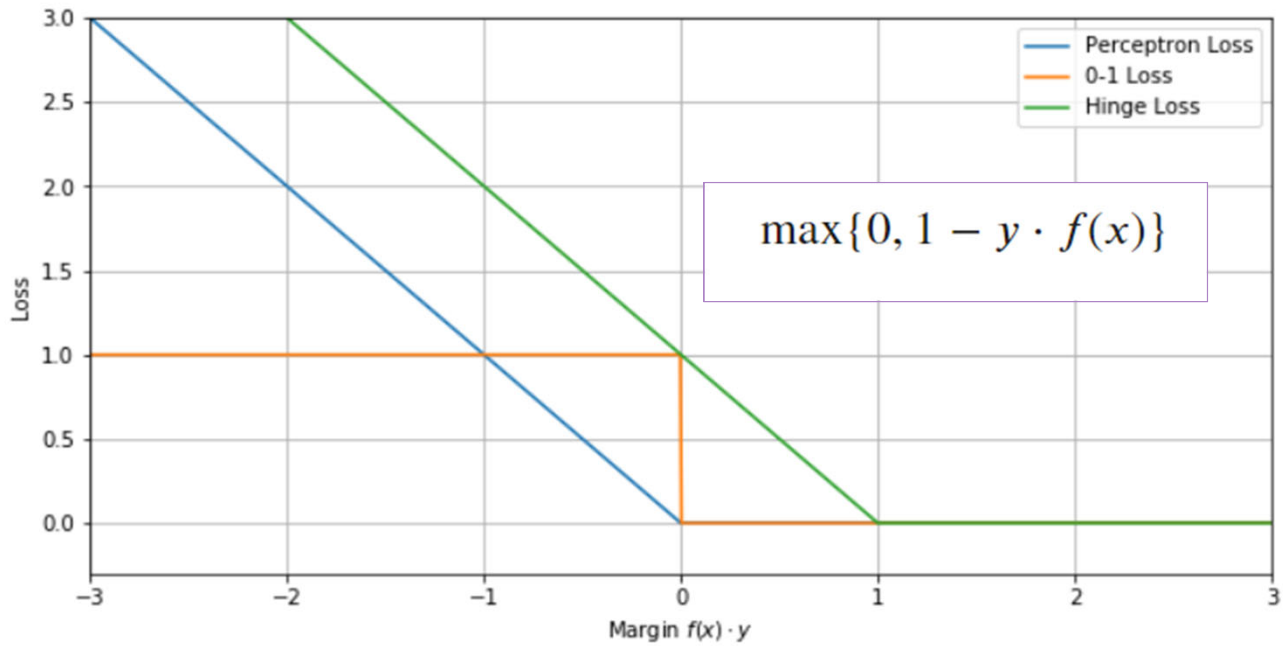
Review

- Minimizing Loss Functions
  - The empirical risk function might lead to optimization errors
  - Approaches
    - Find a replacement loss function



Review

- Minimizing Loss Functions
  - The empirical risk function might lead to optimization errors
  - Approaches
    - Find a replacement loss function
    - Determine another definition for gradient that handles corners

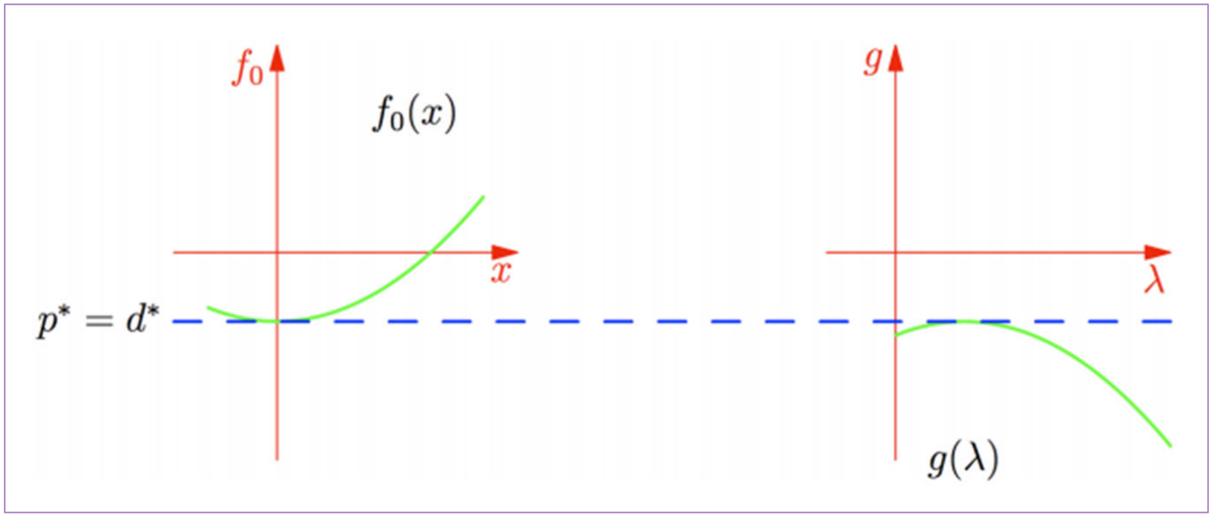


Derivative of hinge loss $\ell(m) = \max(0, 1 - m)$:

$$\ell'(m) = \begin{cases} 0 & m > 1 \\ -1 & m < 1 \\ \text{undefined} & m = 1 \end{cases}$$

Review

- Minimizing Loss Functions
  - The empirical risk function might lead to optimization errors
  - Approaches
    - Rearrange optimization problem
      - Find equivalent problem
      - Combine objective and constraint
      - Switch order of minimization / maximization



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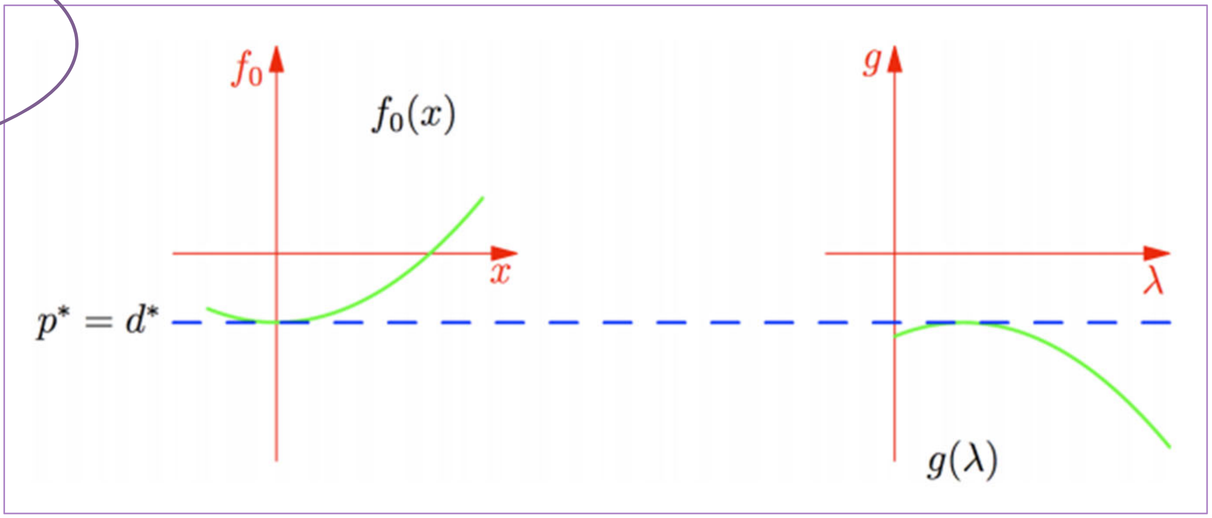

Rearranging Optimization Problems

Question

Suppose we have two functions $f : \mathbf{R}^d \to \mathbf{R}$ and $g : \mathbf{R}^d \to \mathbf{R}$. Now consider the following optimization problem:

$$\boxed{\min_{x \in \mathbf{R}^d} f(x) + g(x).}$$

This is an unconstrained optimization problem. Let's also consider the following constrained optimization problem:

$$\boxed{\begin{array}{ll} \text{minimize} & f(x) + \xi \\ \text{subject to} & \xi \geq g(x). \end{array}}$$

Need to go both ways to have equivalent problem…there cannot be a gap

Review

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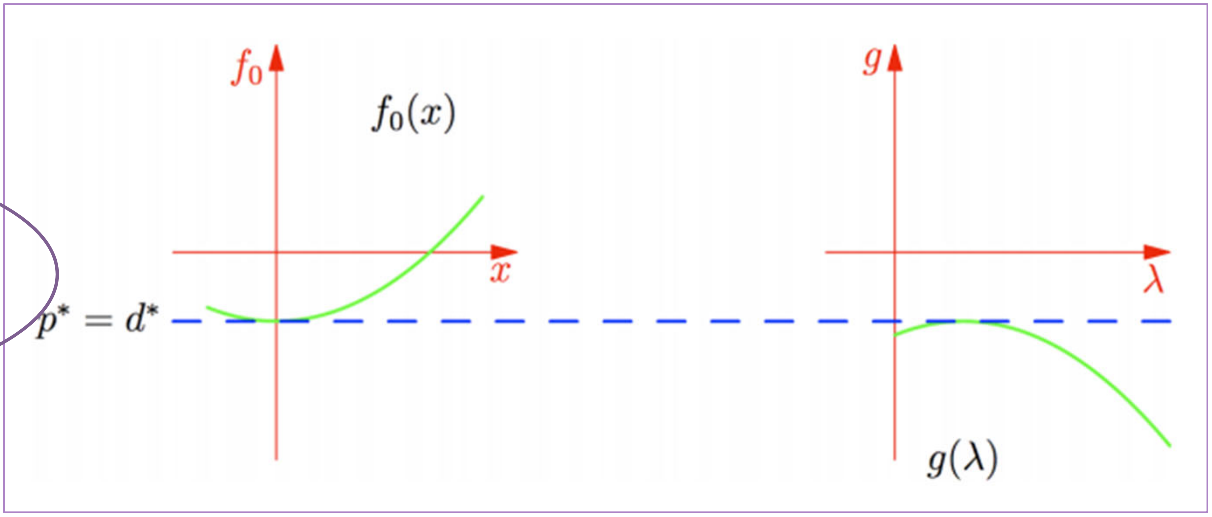

Review

Question

Each row is a student strategy

$$A = \begin{bmatrix} 5 & 5 & 5 & 5 & 5 \\ 8 & 8 & 1 & 8 & 8 \\ +\infty & +\infty & +\infty & 0 & +\infty \end{bmatrix}$$

The entries represent points lost on the assignment

Each column is a grader strategy

Review

Question

$$A = \begin{bmatrix} 5 & 5 & 5 & 5 & 5 \\ 8 & 8 & 1 & 8 & 8 \\ +\infty & +\infty & +\infty & 0 & +\infty \end{bmatrix}$$

- We always have

$$\boxed{\max_j \min_i a_{ij} = d^* \leq p^* = \min_i \max_j a_{ij}.}$$

$$p^* = \min_i \max_j a_{ij}$$

$$d^* = \max_j \min_i a_{ij}$$

Review

Example

$$A = \begin{bmatrix} 5 & 5 & 5 & 5 & 5 \\ 8 & 8 & 1 & 8 & 8 \\ +\infty & +\infty & +\infty & 0 & +\infty \end{bmatrix}$$

- We always have

$$\boxed{\max_j \min_i a_{ij} = d^* \leq p^* = \min_i \max_j a_{ij}.}$$

$$p^* = \min_i \max_j a_{ij}$$

$$d^* = \max_j \min_i a_{ij}$$

because

$$d^* = a_{i_d j_d} \leq a_{i_p j_d} \leq a_{i_p j_p} = p^*.$$

Review

Example

$$A = \begin{bmatrix} 5 & 5 & 5 & 5 & 5 \\ 8 & 8 & 1 & 8 & 8 \\ +\infty & +\infty & +\infty & 0 & +\infty \end{bmatrix}$$

Primal Problem and Dual Problem may not be equal meaning you cannot switch max and min

$$p^* = \min_i \max_j a_{ij}$$

$$d^* = \max_j \min_i a_{ij}$$

- We always have

$$\boxed{\max_j \min_i a_{ij} = d^* \leq p^* = \min_i \max_j a_{ij}.}$$

because

$$d^* = a_{i_d j_d} \leq a_{i_p j_d} \leq a_{i_p j_p} = p^*.$$

Review

The combination is the ***Lagrangian***

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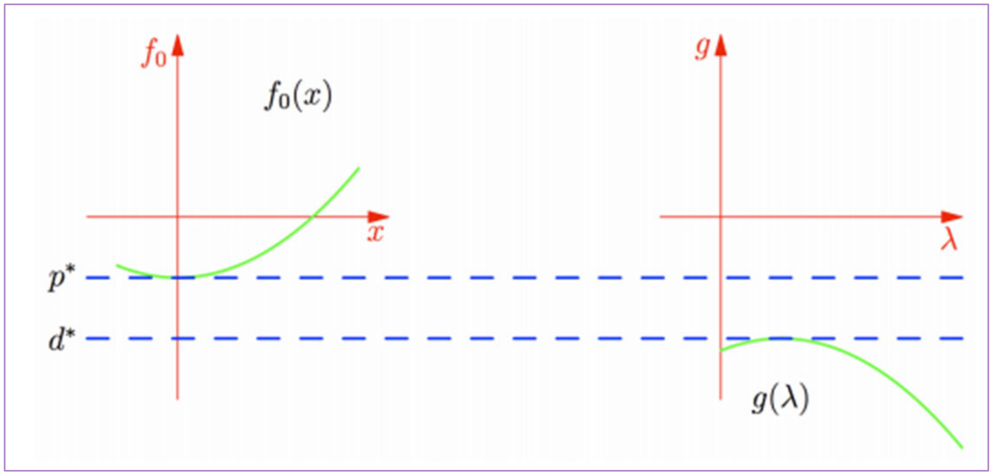

Review

Switching between primal and dual is called ***Lagrangian duality***

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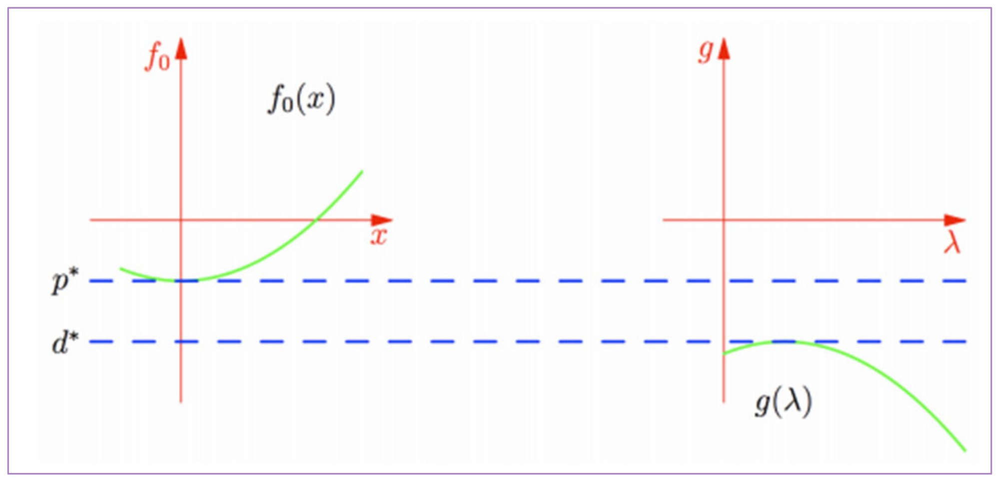

Review

Question

- Minimize $x + y$ subject to constraint $x^2 + y^2 = 1$

Review

Question

- Minimize $x + y$ subject to constraint $x^2 + y^2 = 1$
- We can combine the objective and constraint into a single function is Lagrangian

$$L(x, y, \lambda) = x + y + \lambda(x^2 + y^2 - 1)$$

We call this the ***Lagrange multiplier***…or ***dual variable*** in the context of Lagrangian duality

Review

Question

- Minimize $x + y$ subject to constraint $x^2 + y^2 = 1$
- We can combine the objective and constraint into a single function called the Lagrangian

$$\boxed{L(x, y, \lambda) = x + y + \lambda(x^2 + y^2 - 1)}$$

- Take derivative to find minimum

$$\nabla L = \begin{pmatrix} \frac{\partial L}{\partial x} \\ \frac{\partial L}{\partial y} \\ \frac{\partial L}{\partial \lambda} \end{pmatrix} = \begin{pmatrix} 1 + 2\lambda x \\ 1 + 2\lambda y \\ x^2 + y^2 - 1 \end{pmatrix}$$

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- Solutions at

$$\left(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right) \text{ and } \left(-\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right).$$

Review

Question

- Minimize $x + y$ subject to constraint $x^2 + y^2 \leq 1$

Review

Question

- Minimize $x + y$ subject to constraint $x^2 + y^2 \leq 1$
- We can combine the objective and constraint into a single function the Lagrangian

$$\boxed{L(x, y, \lambda) = x + y + \lambda\left(1 - (x^2 + y^2)\right)}$$

- Here $\lambda > 0$

Review

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Take max over the dual variables and min over the primal variables

Question

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So penalization form and constraint form are definitely the same!

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Note that solutions not unique. Is the objective convex? Is the objective concave?

- Solutions at

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$$\left(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right) \text{ and } \left(-\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right).$$

At the minimizer the constraint is satisfied…this is example of complementary slackness

Agenda

- Lesson
  - Support Vector Machines
    - Hard Margin
    - Dual problem
  - Kernels
    - Relationships between features
- Demo
  - libSVM package for SMO

Objectives

- What is the geometric interpretation of SVM?
- What insights can we gain from the dual formulation of SVM?
- Why would kernels be helpful with many features?
- **Readings:**
  - Shalev-Schwarz Chapter 16
  - Murphy Chapter 14.5 (see 14.5.2.4 for multiclass classification)

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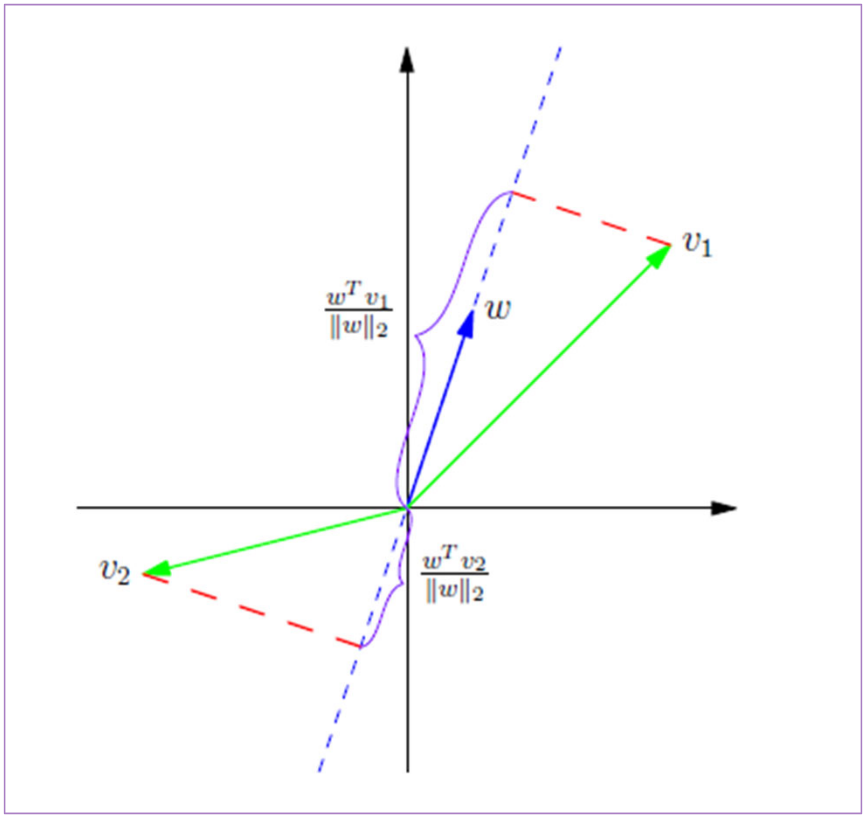
Support Vector Machines

Hard Margin

- A vector determines a plane in space. It consists of vectors at a right angle.
- Note that scaling the vector yields the same plane of perpendicular vectors



Support Vector Machines

Hard Margin

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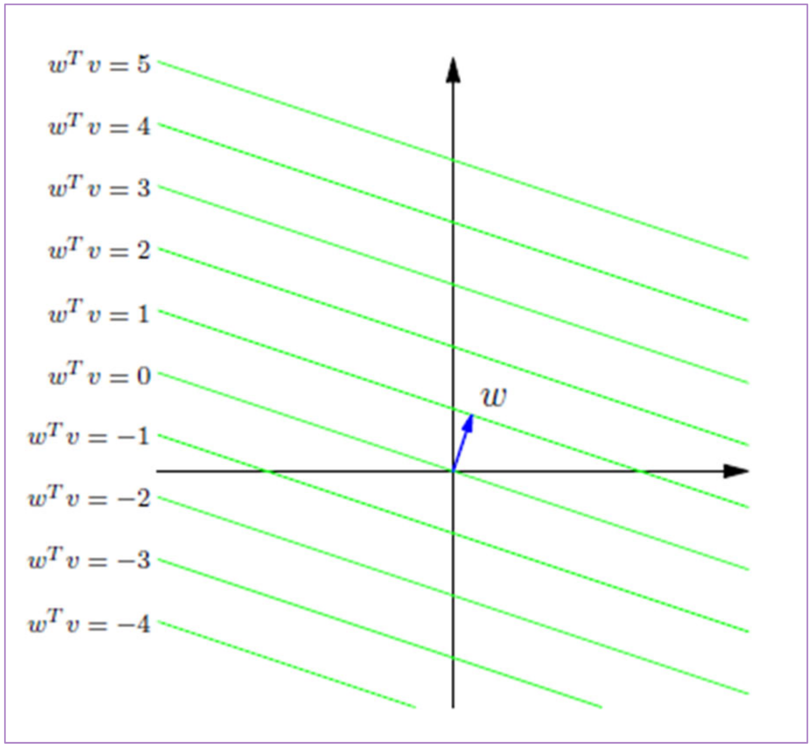
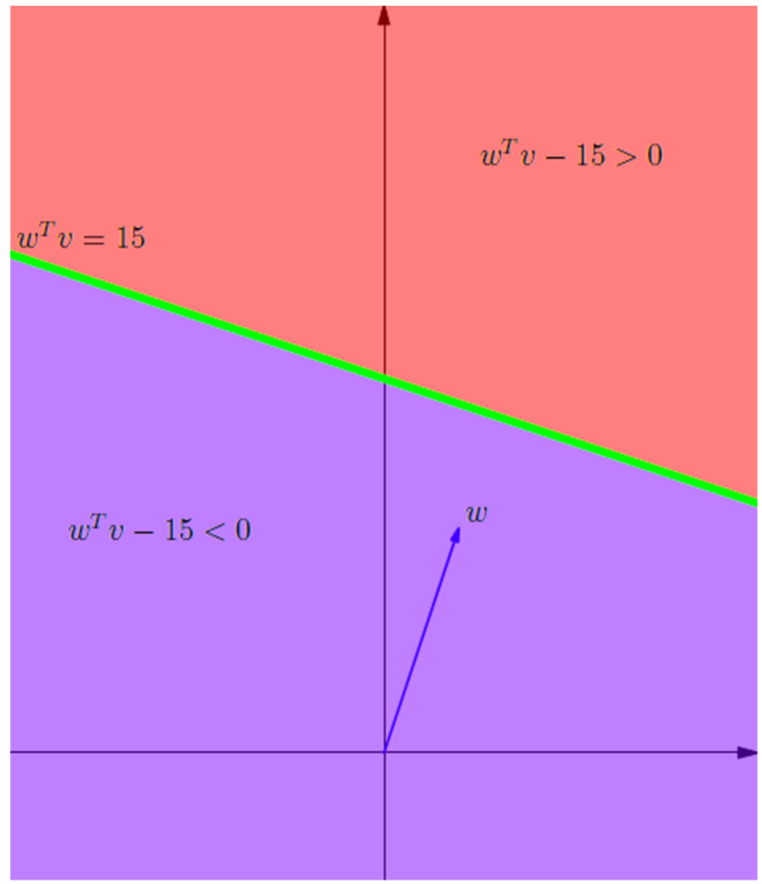
- Note that scaling the vector yields the same plane of perpendicular vectors
- The offset term b determine shift up or down



Hard Margin

Support Vector Machines

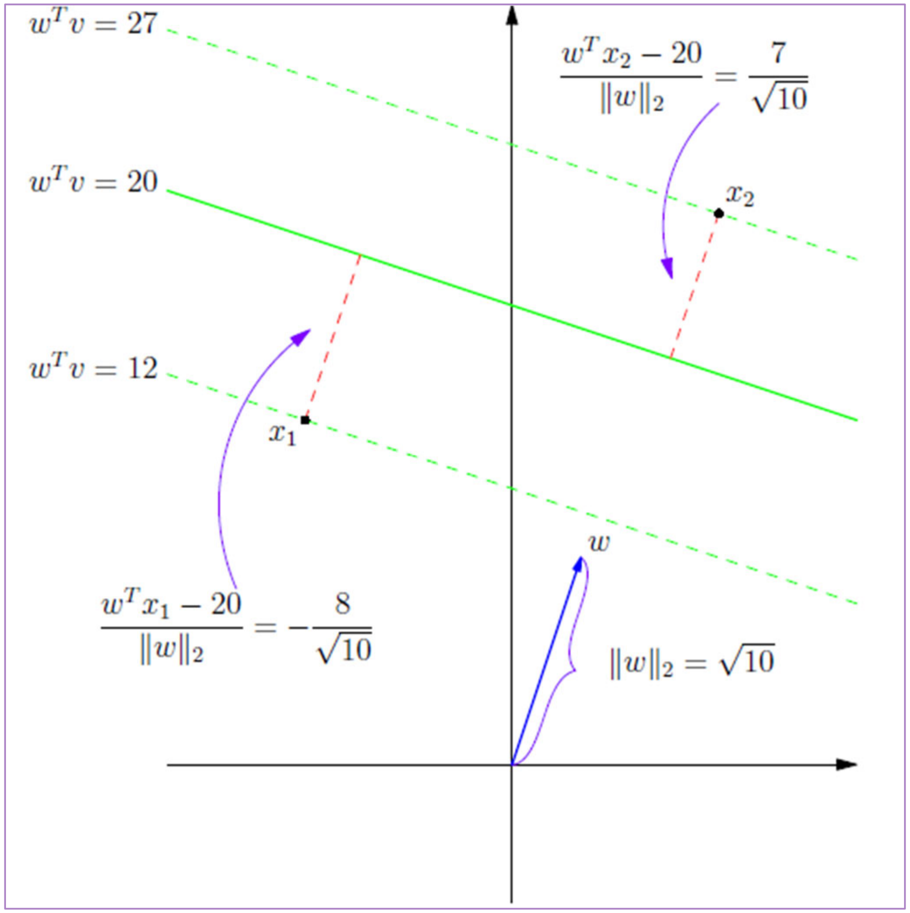
- Note that distance from the plane has a sign…
  - Positive for above the plane
  - Negative for below the plane



Support Vector Machines

Hard Margin

- Note that distance from the plane has a sign…
  - Positive for above the plane
  - Negative for below the plane
- The ***geometric margin*** gives the signed distance from the plane
  - Note the term in the denominator is different from the (functional) margin

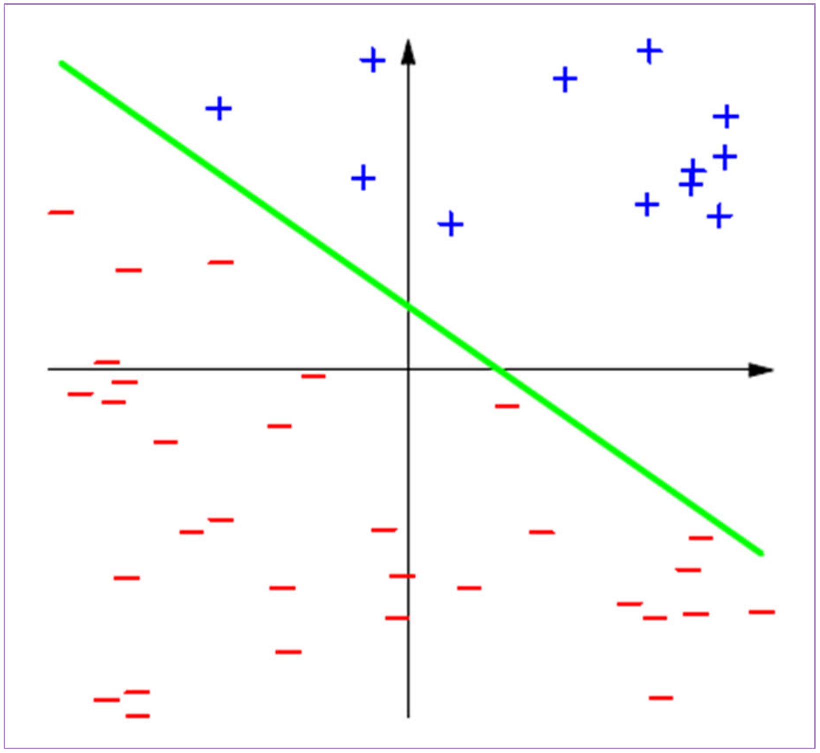


Support Vector Machines

Hard Margin

- We want to classify points in the training set with a separating plane.
  - Here the hypothesis set consists of functions

$$\mathrm{sgn}(w^T x + a).$$



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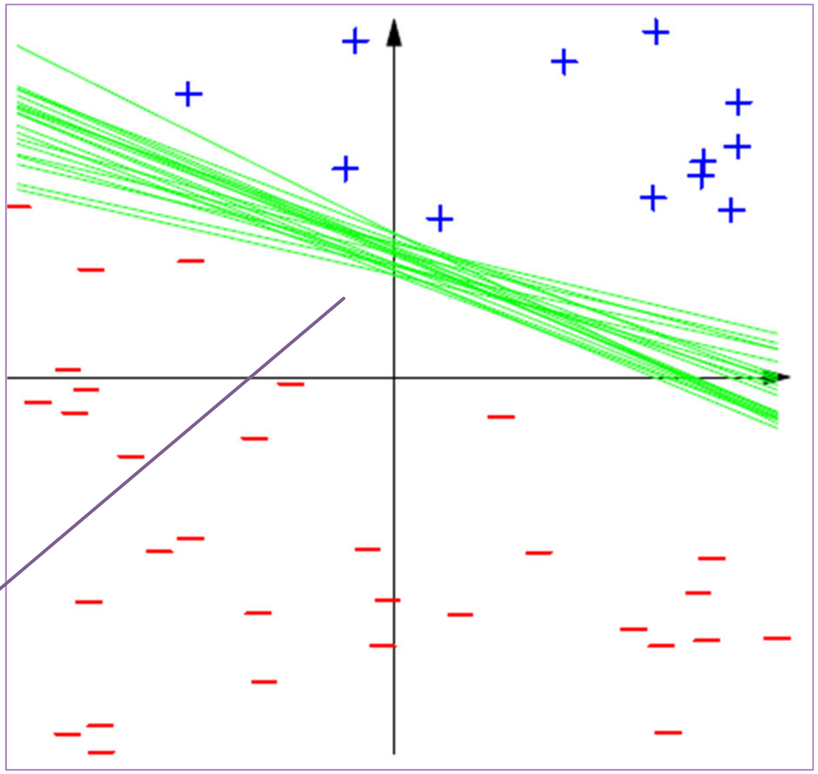
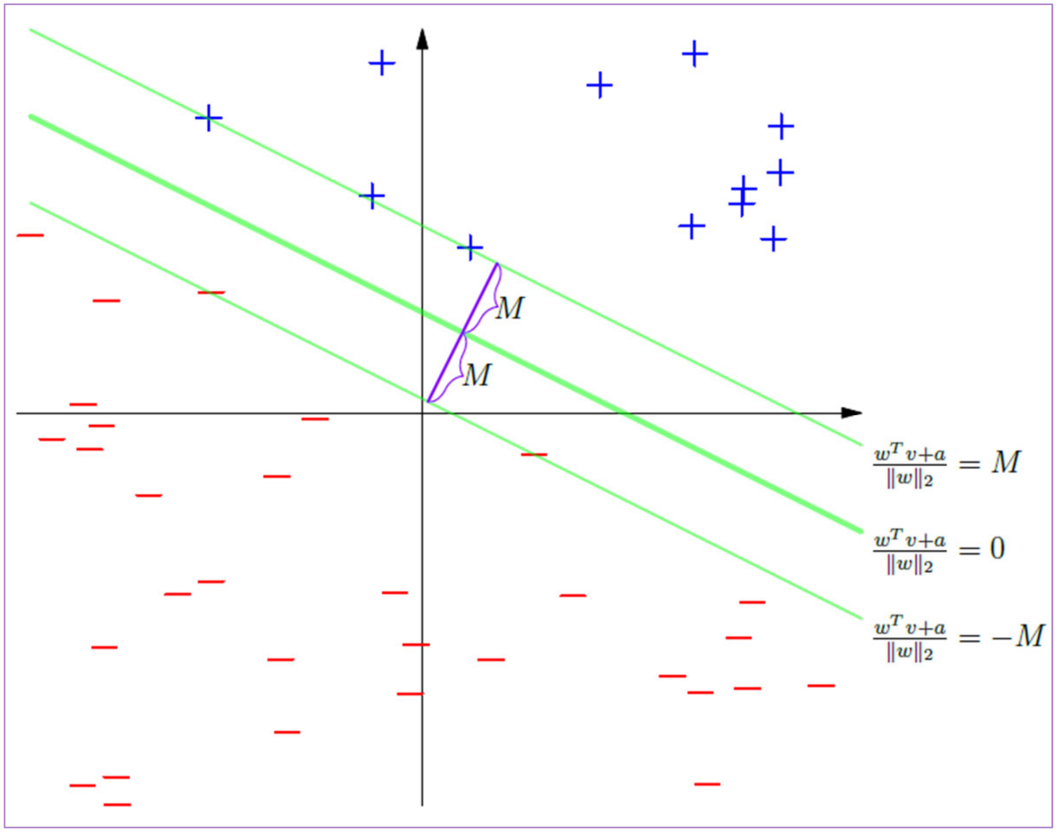


This was a problem with Perceptron…could lead to overfitting

Hard Margin

Support Vector Machines

- We want to classify points in the training set with a separating plane.
  - We can incorporate confidence into the hypotheses with the geometric margin

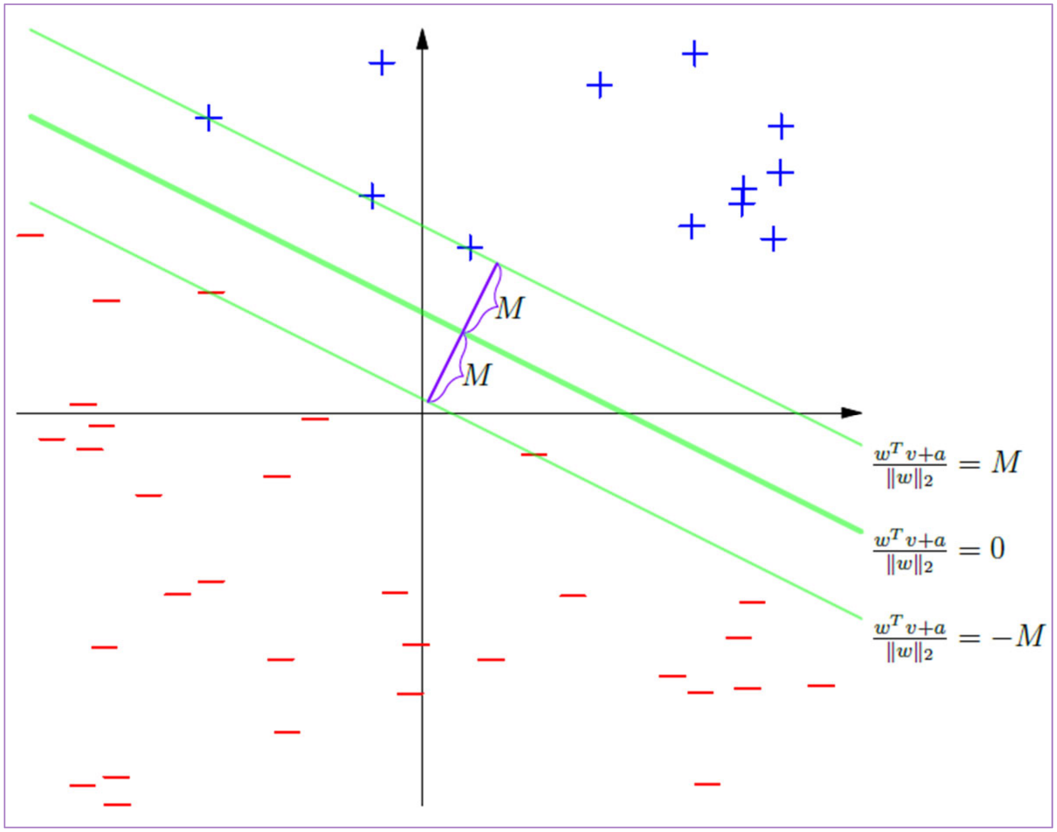


Support Vector Machines

Hard Margin

- We want to classify points in the training set with a separating plane.
  - We can incorporate confidence into the hypotheses with the geometric margin
  - Distance from plane is

$$\left| \frac{w^T x_i + a}{\|w\|_2} \right| = \frac{y_i(w^T x_i + a)}{\|w\|_2}$$



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$$\boxed{\left|\frac{w^T x_i + a}{\|w\|_2}\right| = \frac{y_i(w^T x_i + a)}{\|w\|_2}}$$

Goal

$$\text{maximize}_{w,a} \quad \min_i \frac{y_i(w^T x_i + a)}{\|w\|_2}.$$

Support Vector Machines

Hard Margin

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$$\boxed{\left|\frac{w^T x_i + a}{\|w\|_2}\right| = \frac{y_i(w^T x_i + a)}{\|w\|_2}}$$

Goal

$$\text{maximize}_{w,a} \quad \min_i \frac{y_i(w^T x_i + a)}{\|w\|_2}.$$

Rearrange to equivalent problem

$$\begin{aligned} &\text{maximize}_{w,a,M} && M \\ &\text{subject to} && \frac{y_i(w^T x_i + a)}{\|w\|_2} \geq M \quad \text{for all } i \end{aligned}$$

Support Vector Machines

Hard Margin

- We want to classify points in the training set with a separating plane.
  - We can incorporate confidence into the hypotheses with the geometric margin
  - Distance from plane is

$$\boxed{\left|\frac{w^T x_i + a}{\|w\|_2}\right| = \frac{y_i(w^T x_i + a)}{\|w\|_2}}$$

Goal

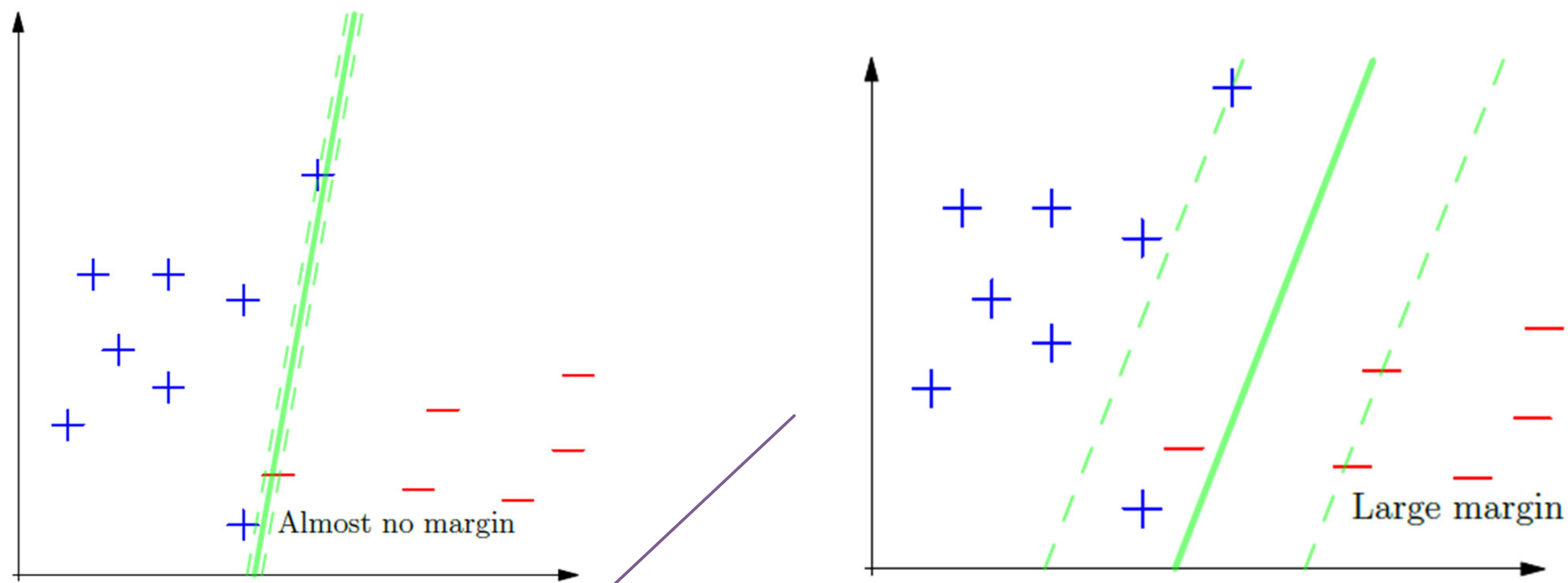
$$\begin{aligned} &\text{maximize}_{w,a,M} && M \\ &\text{subject to} && \frac{y_i(w^T x_i + a)}{\|w\|_2} \geq M \quad \text{for all } i \end{aligned}$$

Rearrange to equivalent problem

$$\begin{aligned} &\text{maximize}_{w,a} && 1/\|w\|_2 \\ &\text{subject to} && y_i(w^T x_i + a) \geq 1 \quad \text{for all } i \end{aligned}$$

Support Vector Machines

Hard Margin



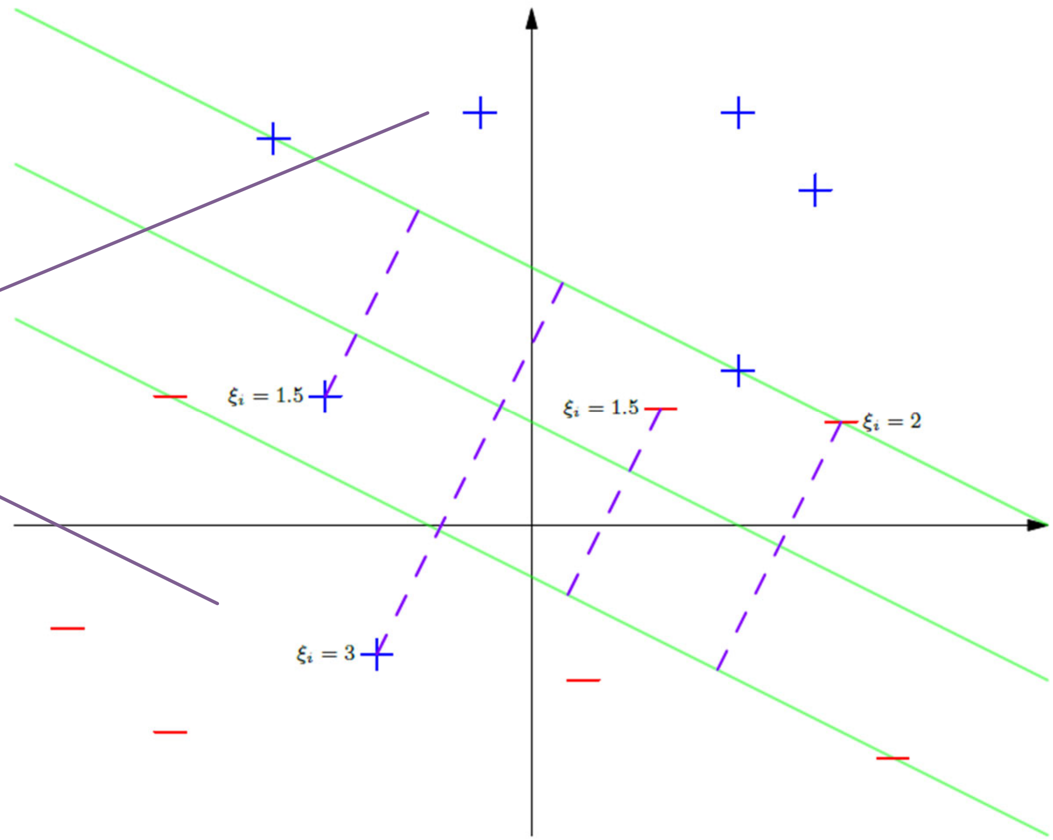
Which separating plan will better generalize from in-sample to out-of-sample?

Support Vector Machines

Soft Margin

Allow for violations for the constraint...instead use penalization

Slack variable is 0 for correctly classified points



Support Vector Machines

Soft Margin

- We can avoid overfitting through relaxation of the constraint.
- We switch from constraint form to penalization form

Goal

$$\begin{array}{ll} \text{minimize}_{w,a} & \|w\|_2^2 \\ \text{subject to} & y_i(w^T x_i + a) \geq 1 \quad \text{for all } i \end{array}$$

Rearrange to equivalent problem

$$\begin{array}{ll} \text{minimize}_{w,a,\xi} & \|w\|_2^2 + \frac{C}{n}\sum_{i=1}^n \xi_i \\ \text{subject to} & y_i(w^T x_i + a) \geq 1 - \xi_i \quad \text{for all } i \\ & \xi_i \geq 0 \quad \text{for all } i. \end{array}$$

Support Vector Machines

Soft Margin

$$\begin{aligned}
&\text{minimize} && \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i \\
&\text{subject to} && \xi_i \geqslant \left(1 - y_i \left[w^T x_i + b\right]\right) \text{ for } i = 1, \ldots, n \\
& && \xi_i \geqslant 0 \text{ for } i = 1, \ldots, n
\end{aligned}$$

Differentiable with n + d + 1 unknowns

Support Vector Machines

Soft Margin

$$\text{minimize} \quad \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i$$

$$\text{subject to} \quad \xi_i \geqslant \max\left(0, 1 - y_i\left[w^T x_i + b\right]\right).$$

$$\text{minimize} \quad \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i$$

$$\text{subject to} \quad \xi_i \geqslant \left(1 - y_i\left[w^T x_i + b\right]\right) \text{ for } i = 1, \ldots, n$$

$$\xi_i \geqslant 0 \text{ for } i = 1, \ldots, n$$

Differentiable with n + d + 1 unknowns

Support Vector Machines

Soft Margin

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i\left[w^T x_i + b\right]\right).$$

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i \\ \text{subject to} & \xi_i \geqslant \max\left(0, 1 - y_i\left[w^T x_i + b\right]\right). \end{array}$$

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Differentiable with n + d + 1 unknowns

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$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i\left[w^T x_i + b\right]\right).$$

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Quadratic Programming Problem…could solve with CVXOPT

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i \\ \text{subject to} & \xi_i \geqslant \left(1 - y_i\left[w^T x_i + b\right]\right) \text{ for } i = 1, \ldots, n \\ & \xi_i \geqslant 0 \text{ for } i = 1, \ldots, n \end{array}$$

Differentiable with n + d + 1 unknowns

Support Vector Machines

Soft Margin

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i \left[w^T x_i + b\right]\right).$$

Support Vector Machines

Soft Margin

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i\left[w^T x_i + b\right]\right).$$

Penalization form not constraint form with l2 regularization not l1 regularization

Support Vector Machines

Soft Margin

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}||w||^2 + \frac{c}{n} \sum_{i=1}^{n} \max\left(0, 1 - y_i \left[w^T x_i + b\right]\right).$$

c not lambda

Penalization form not constraint form with l2 regularization not l1 regularization

Support Vector Machines

Soft Margin

b is intercept term in line…for classification with lines b is threshold

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}||w||^2 + \frac{c}{n} \sum_{i=1}^{n} \max\left(0, 1 - y_i \left[w^T x_i + b\right]\right).$$

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Support Vector Machines

Soft Margin

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$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i\left[w^T x_i + b\right]\right).$$

c not lambda

Measures the confidence of the prediction, that is, the margin

Penalization form not constraint form with l2 regularization not l1 regularization

Measures the accuracy of the classification

Demo

- Support Vector Machine
  - Iris Dataset
  - Features
    - Petal Width
    - Petal Length
  - Classification
    - Iris-Versicolor
    - Iris-Setosa

Take-Aways

- Why is SVM affected by scaling?
- How can soft margin SVM be used to detect outliers?
- How does changing C affect the classification? What prevents against overfitting.
- How do we use SVM in sklearn?

Agenda

- Lesson
  - Support Vector Machines
    - Hard Margin
    - Dual problem
  - Kernels
    - Relationships between features
- Demo
  - libSVM package for SMO

Objectives

- What is the geometric interpretation of SVM?
- **What insights can we gain from the dual formulation of SVM?**
- Why would kernels be helpful with many features?
- **Readings:**
  - Shalev-Schwarz Chapter 16
  - Murphy Chapter 14.5 (see 14.5.2.4 for multiclass classification)

Support Vector Machines

Dual Problem

- If we form the Lagrangian, then we can incorporate maximization into the minimization problem

$$
\begin{array}{ll}
\text{minimize} & \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i \\
\text{subject to} & -\xi_i \leqslant 0 \text{ for } i = 1, \ldots, n \\
& \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1, \ldots, n
\end{array}
$$

Support Vector Machines

Dual Problem

- If we form the Lagrangian, then we can incorporate maximization into the minimization problem

$$
\begin{aligned}
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& \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1,\ldots,n
\end{aligned}
$$

Lagrange Multiplier	Constraint
λ_i	$-\xi_i \leqslant 0$
α_i	$\left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0$

Dual Problem

Support Vector Machines

- If we form the Lagrangian, then we can incorporate maximization into the minimization problem

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i \\ \text{subject to} \quad & -\xi_i \leqslant 0 \text{ for } i = 1, \dots, n \\ & \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1, \dots, n \end{aligned}$$

Lagrange Multiplier	Constraint
λ_i	$-\xi_i \leqslant 0$
α_i	$\left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0$

$$L(w, b, \xi, \alpha, \lambda) = \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i + \sum_{i=1}^{n} \alpha_i \left(1 - y_i\left[w^T x_i + b\right] - \xi_i\right) + \sum_{i=1}^{n} \lambda_i (-\xi_i)$$

Support Vector Machines

Dual Problem

- If we form the Lagrangian, then we can incorporate maximization into the minimization problem

$$\begin{aligned} p^* &= \inf_{w,\xi,b} \sup_{\alpha,\lambda\succeq 0} L(w,b,\xi,\alpha,\lambda) \\ &\geqslant \sup_{\alpha,\lambda\succeq 0} \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda) = d^* \end{aligned}$$

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\ \text{subject to} \quad & -\xi_i \leqslant 0 \text{ for } i = 1,\dots,n \\ & \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1,\dots,n \end{aligned}$$

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λ_i	$-\xi_i \leqslant 0$
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Support Vector Machines

Dual Problem

- While primal problem and dual problem may not be equivalent, we are able to check ***constraint qualifications*** that guarantee equivalence

$$
\begin{aligned}
p^* &= \inf_{w,\xi,b} \sup_{\alpha,\lambda \succeq 0} L(w,b,\xi,\alpha,\lambda) \\
&\geqslant \sup_{\alpha,\lambda \succeq 0} \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda) = d^*
\end{aligned}
$$

$$
\begin{aligned}
\text{minimize} \quad & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n} \xi_i \\
\text{subject to} \quad & -\xi_i \leqslant 0 \text{ for } i = 1,\ldots,n \\
& \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1,\ldots,n
\end{aligned}
$$

Lagrange Multiplier	Constraint
λ_i	$-\xi_i \leqslant 0$
α_i	$\left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0$

$$
L(w,b,\xi,\alpha,\lambda) = \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\alpha_i\left(1 - y_i\left[w^T x_i + b\right] - \xi_i\right) + \sum_{i=1}^{n}\lambda_i(-\xi_i)
$$

Support Vector Machines

Dual Problem

- While primal problem and dual problem may not be equivalent, we are able to check ***constraint qualifications*** that guarantee equivalence

$$p^* = \inf_{w,\xi,b} \sup_{\alpha,\lambda\succeq 0} L(w,b,\xi,\alpha,\lambda)$$
$$= \sup_{\alpha,\lambda\succeq 0} \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda) = d^*$$

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\ \text{subject to} & -\xi_i \leqslant 0 \text{ for } i = 1,\dots,n \\ & \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1,\dots,n \end{array}$$

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$$L(w,b,\xi,\alpha,\lambda) = \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\alpha_i\left(1 - y_i\left[w^T x_i + b\right] - \xi_i\right) + \sum_{i=1}^{n}\lambda_i(-\xi_i)$$

Support Vector Machines

Dual Problem

- With the dual problem, we have to maximize...

$$g(\alpha,\lambda) = \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda)$$

$$= \inf_{w,b,\xi}\left[\frac{1}{2}w^Tw + \sum_{i=1}^{n}\xi_i\left(\frac{c}{n}-\alpha_i-\lambda_i\right)+\sum_{i=1}^{n}\alpha_i\left(1-y_i\left[w^Tx_i+b\right]\right)\right]$$

Support Vector Machines

Dual Problem

- With the dual problem, we have to maximize…

$$g(\alpha,\lambda) = \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda)$$

$$= \inf_{w,b,\xi} \left[\frac{1}{2} w^T w + \sum_{i=1}^{n} \xi_i \left(\frac{c}{n} - \alpha_i - \lambda_i \right) + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \left[w^T x_i + b \right] \right) \right]$$

- What does the derivative tell us about the minimum?
  - Note that the weight, offset and slack are unconstrainted so we have no trouble taking derivatives

Support Vector Machines

Dual Problem

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$$g(\alpha,\lambda) = \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda)$$

$$= \inf_{w,b,\xi}\left[\frac{1}{2}w^T w + \sum_{i=1}^{n}\xi_i\left(\frac{c}{n}-\alpha_i-\lambda_i\right)+\sum_{i=1}^{n}\alpha_i\left(1-y_i\left[w^T x_i+b\right]\right)\right]$$

- What does the derivative tell us about the minimum?
  - Note that the weight, offset and slack are unconstrainted so we have no trouble taking derivatives

$$\partial_w L = 0 \iff w - \sum_{i=1}^{n}\alpha_i y_i x_i = 0 \iff \boxed{w = \sum_{i=1}^{n}\alpha_i y_i x_i}$$

Support Vector Machines

Dual Problem

- With the dual problem, we have to maximize…

$$g(\alpha,\lambda) = \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda)$$

$$= \inf_{w,b,\xi}\left[\frac{1}{2}w^T w + \sum_{i=1}^{n}\xi_i\left(\frac{c}{n}-\alpha_i-\lambda_i\right)+\sum_{i=1}^{n}\alpha_i\left(1-y_i\left[w^T x_i+b\right]\right)\right]$$

- What does the derivative tell us about the minimum?
  - Note that the weight, offset and slack are unconstrainted so we have no trouble taking derivatives

$$\partial_b L = 0 \iff -\sum_{i=1}^{n}\alpha_i y_i = 0 \iff \boxed{\sum_{i=1}^{n}\alpha_i y_i = 0}$$

Support Vector Machines

Dual Problem

- With the dual problem, we have to maximize...

$$g(\alpha, \lambda) = \inf_{w,b,\xi} L(w, b, \xi, \alpha, \lambda)$$

$$= \inf_{w,b,\xi} \left[\frac{1}{2} w^T w + \sum_{i=1}^{n} \xi_i \left(\frac{c}{n} - \alpha_i - \lambda_i \right) + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \left[w^T x_i + b \right] \right) \right]$$

- What does the derivative tell us about the minimum?
  - Note that the weight, offset and slack are unconstrainted so we have no trouble taking derivatives

$$\partial_{\xi_i} L = 0 \iff \frac{c}{n} - \alpha_i - \lambda_i = 0 \iff \boxed{\alpha_i + \lambda_i = \frac{c}{n}}$$

Support Vector Machines

Dual Problem

- Putting it together we obtain, these first order conditions show us that the dual problem is equivalent to

$$
\begin{aligned}
\sup_{\alpha} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_j^T x_i \\
\text{s.t.} \quad & \sum_{i=1}^{n} \alpha_i y_i = 0 \\
& \alpha_i \in \left[0, \frac{c}{n}\right] \quad i = 1, \dots, n.
\end{aligned}
$$

Support Vector Machines

Dual Problem

- Putting it together we obtain, these first order conditions show us that the dual problem is equivalent to

$$\begin{aligned} \sup_{\alpha} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_j{}^T x_i \\ \text{s.t.} \quad & \sum_{i=1}^{n} \alpha_i y_i = 0 \\ & \alpha_i \in \left[0, \frac{c}{n}\right] \quad i = 1, \ldots, n. \end{aligned}$$

The weights come from the dual variables

$$w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i.$$

Support Vector Machines

Dual Problem

- Putting it together we obtain, these first order conditions show us that the dual problem is equivalent to

The hyperparameter limits the size…actually most will be 0

$$\sup_{\alpha} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_j^T x_i$$

$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

$$\alpha_i \in \left[0, \frac{c}{n}\right] \quad i = 1, \ldots, n.$$

The weights come from the dual variables

$$w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i.$$

Support Vector Machines

Dual Problem

- Remember that we have ***complementary slackness*** conditions that relate values of dual variables and constraints

$$\alpha_i^* \left(1 - y_i f^*(x_i) - \xi_i^*\right) = 0$$

$$\lambda_i^* \xi_i^* = \left(\frac{c}{n} - \alpha_i^*\right) \xi_i^* = 0$$

Support Vector Machines

Dual Problem

- Remember that we have ***complementary slackness*** conditions that relate values of dual variables and constraints

$$\alpha_i^* = 0 \implies y_i f^*(x_i) \geqslant 1$$
$$\alpha_i^* \in \left(0, \frac{c}{n}\right) \implies y_i f^*(x_i) = 1$$
$$\alpha_i^* = \frac{c}{n} \implies y_i f^*(x_i) \leqslant 1$$

$$y_i f^*(x_i) < 1 \implies \alpha_i^* = \frac{c}{n}$$
$$y_i f^*(x_i) = 1 \implies \alpha_i^* \in \left[0, \frac{c}{n}\right]$$
$$y_i f^*(x_i) > 1 \implies \alpha_i^* = 0$$

$$\alpha_i^* \left(1 - y_i f^*(x_i) - \xi_i^*\right) = 0$$
$$\lambda_i^* \xi_i^* = \left(\frac{c}{n} - \alpha_i^*\right) \xi_i^* = 0$$

When are the constraints ***active?***

Agenda

- Lesson
  - Support Vector Machines
    - Hard Margin
    - Dual problem
  - Kernels
    - Relationships between features
- Demo
  - libSVM package for SMO

Objectives

- What is the geometric interpretation of SVM?
- What insights can we gain from the dual formulation of SVM?
- Why would kernels be helpful with many features?
- **Readings:**
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Kernels

- The dual problem for SVM just depends on the inner products of the points in the sample
- How could we change to other relationships besides the ***linear kernel***?

$$
\begin{aligned}
\sup_{\alpha} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j {x_j}^T x_i \\
\text{s.t.} \quad & \sum_{i=1}^{n} \alpha_i y_i = 0 \\
& \alpha_i \in \left[0, \frac{c}{n}\right] \; i = 1, \ldots, n.
\end{aligned}
$$

Kernels

Example

- Consider feature encoding for strings representing amino acids.
  - The characters are $\{A, R, N, D, C, E, Q, G, H, I, L, K, M, F, P, S, T, W, Y, V\}$

Kernels

Example

- Consider feature encoding for strings representing amino acids.
  - The characters are $\boxed{\{A, R, N, D, C, E, Q, G, H, I, L, K, M, F, P, S, T, W, Y, V\}}$
- How should we relate the following strings…

```
IPTSALVKETLALLSTHRTLLIANETLRIPVPVHKNHQLCTEEIFQGIGTLESQTVQGGTV
ERLFKNLSLIKKYIDGQKKKCGEERRRVNQFLDYLQEFLGVMNTEWI
```

```
PHRRDLCSRSIWLARKIRSDLTALTESYVKHQGLWSELTEAERLQENLQAYRTFHVLLA
RLLEDQQVHFTPTEGDFHQAIHTLLLQVAAFAYQIEELMILLEYKIPRNEADGMLFEKK
LWGLKVLQELSQWTVRSIHDLRFISSHQTGIP
```

Kernels

Example

- Consider feature encoding for strings representing amino acids.
  - The characters are $\boxed{\{A, R, N, D, C, E, Q, G, H, I, L, K, M, F, P, S, T, W, Y, V\}}$
- How should we relate the following strings…

```
IPTSALVKETLALLSTHRTLLIANETLRIPVPVHKNHQLCTEEIFQGIGTLESQTVQGGTV
ERLFKNLSLIKKYIDGQKKKCGEERRRVNQFLDYLQEFLGVMNTEWI
```

$$\boxed{\kappa(x, x') = \sum_{s \in \mathcal{A}^*} w_s \phi_s(x) \phi_s(x')}$$

```
PHRRDLCSRSIWLARKIRSDLTALTESYVKHQGLWSELTEAERLQENLQAYRTFHVLLA
RLLEDQQVHFTPTEGDFHQAIHTLLLQVAAFAYQIEELMILLEYKIPRNEADGMLFEKK
LWGLKVLQELSQWTVRSIHDLRFISSHQTGIP
```

Summary

- Support Vector Machines
  - Hard Margin: Only applies to linearly separable data
  - Soft Margin: Allows for slack variables. Useful for outlier detection
- Rearranging Optimization Problems
  - Combine objective and constraint
  - Switch order of minimization / maximization
  - Lagrangians, First Order Conditions and Complementary Slackness
- Kernels
  - Replace features with relationships between features
  - We can use kernels for SVM because the problem depends on inner products – the linear kernel