Support Vector Machine

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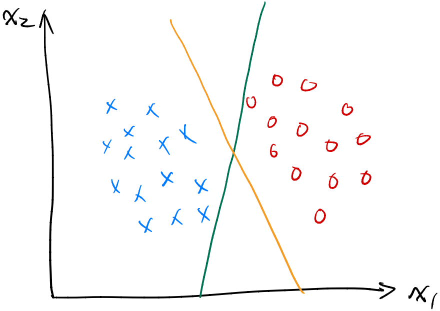
Maximum-Margin Separating Hyperplane

For separable data, there are infinitely many zero-error classifiers.

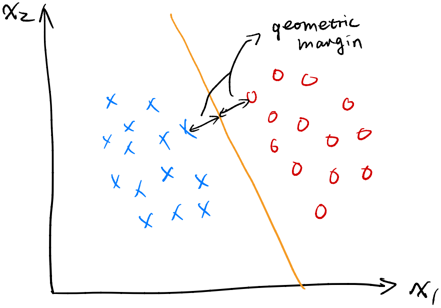
Which one do we pick?



(Perceptron does not return a unique solution.)

Maximum-Margin Separating Hyperplane

We prefer the classifier that is farthest from both classes of points



- Geometric margin: smallest distance between the hyperplane and the points
- Maximum margin: *largest* distance to the closest points

Geometric Margin

We want to maximize the distance between the separating hyperplane and the closest points.

Let's formalize the problem.

Definition (separating hyperplane)

We say (x_i, y_i) for $i = 1, \ldots, n$ are **linearly separable** if there is a $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$ such that $y_i(w^T x_i + b) > 0$ for all i. The set $\{v \in \mathbb{R}^d \mid w^T v + b = 0\}$ is called a **separating hyperplane**.

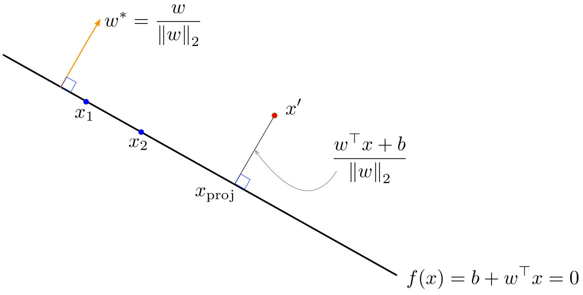
Definition (geometric margin)

Let H be a hyperplane that separates the data (x_i, y_i) for $i = 1, \ldots, n$. The **geometric margin** of this hyperplane is

$$\min_i d(x_i, H),$$

the distance from the hyperplane to the closest data point.

Distance between a Point and a Hyperplane



Maximize the Margin

We want to maximize the geometric margin:

$$\text{maximize} \min_i d(x_i, H).$$

Given separating hyperplane $H = \left\{v \mid w^T v + b = 0\right\}$, we have

$$\text{maximize} \min_i \frac{y_i(w^T x_i + b)}{\|w\|_2}.$$

Let's remove the inner minimization problem by

$$\begin{array}{ll} \text{maximize} & M \\ \text{subject to} & \frac{y_i(w^T x_i + b)}{\|w\|_2} \geqslant M \quad \text{for all } i \end{array}$$

Note that the solution is not unique (why?).

Maximize the Margin

Let's fix the norm $\|w\|_2$ to $1/M$ to obtain:

$$\begin{array}{ll} \text{maximize} & \frac{1}{\|w\|_2} \\ \text{subject to} & y_i(w^T x_i + b) \geqslant 1 \quad \text{for all } i \end{array}$$

It's equivalent to solving the minimization problem

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

Note that $y_i(w^T x_i + b)$ is the (functional) margin. The optimization finds the minimum norm solution which has a margin of at least 1 on all examples.

Not linearly separable

What if the data is *not* linearly separable?

For any w, there will be points with a negative margin.

Soft Margin SVM

Introduce **slack variables** ξ's to penalize small margin:

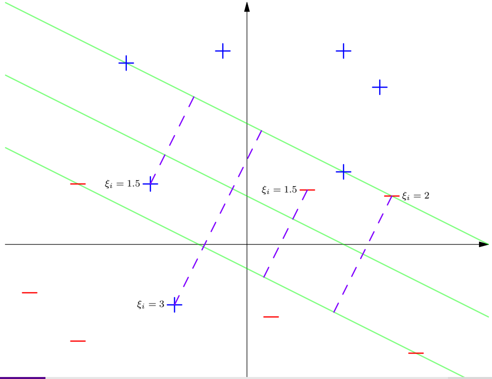
$$
\begin{array}{ll}
\text{minimize} & \frac{1}{2}\|w\|_2^2 + \frac{C}{n}\sum_{i=1}^n \xi_i \\
\text{subject to} & y_i(w^T x_i + b) \geqslant 1 - \xi_i \quad \text{for all } i \\
& \xi_i \geqslant 0 \quad \text{for all } i
\end{array}
$$

- If $\xi_i = 0 \; \forall i$, it's reduced to hard SVM.
- What does $\xi_i > 0$ mean?
- What does C control?

Slack Variables

$d(x_i, H) = \frac{y_i(w^T x_i + b)}{\|w\|_2} \geqslant \frac{1-\xi_i}{\|w\|_2}$, thus ξ_i measures the violation by multiples of the geometric margin:

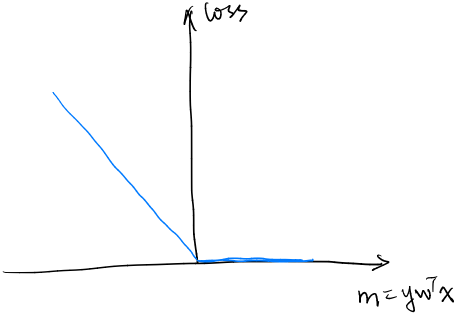
- $\xi_i = 1$: x_i lies on the hyperplane
- $\xi_i = 3$: x_i is past 2 margin width beyond the decision hyperplane



Minimize the Hinge Loss

Perceptron Loss

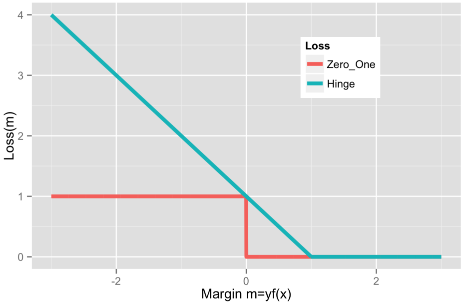
$$\ell(x, y, w) = \max(0, -yw^T x)$$



If we do ERM with this loss function, what happens?

Hinge Loss

- SVM/Hinge loss: $\ell_{\text{Hinge}} = \max\{1-m, 0\} = (1-m)_+$
- Margin $m = yf(x)$; "Positive part" $(x)_+ = x\mathbb{1}[x \geqslant 0]$.



Hinge is a **convex**, **upper bound** on $0-1$ loss. Not differentiable at $m=1$.
We have a **"margin error"** when $m<1$.

SVM as an Optimization Problem

- The SVM optimization problem is equivalent to

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

which is equivalent to

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

SVM as an Optimization Problem

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

Move the constraint into the objective:

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

- The first term is the L2 regularizer.
- The second term is the Hinge loss.

Support Vector Machine

Using ERM:

- Hypothesis space $\mathcal{F} = \left\{ f(x) = w^T x + b \mid w \in \mathrm{R}^d, b \in \mathrm{R} \right\}$.
- ℓ_2 regularization (Tikhonov style)
- Hinge loss $\ell(m) = \max\{1-m, 0\} = (1-m)_+$
- The SVM prediction function is the solution to

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

Summary

Two ways to derive the SVM optimization problem:

- Maximize the margin
- Minimize the hinge loss with ℓ_2 regularization

Both leads to the minimum norm solution satisfying certain margin constraints.

- **Hard-margin SVM**: all points must be correctly classified with the margin constraints
- **Soft-margin SVM**: allow for margin constraint violation with some penalty

SVM Optimization Problem

- SVM objective function:

$$J(w) = \frac{1}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i w^T x_i\right) + \lambda \|w\|^2.$$

- Not differentiable... but let's think about gradient descent anyway.
- Hinge loss: $\ell(m) = \max(0, 1-m)$

$$\begin{aligned}
\nabla_w J(w) &= \nabla_w \left(\frac{1}{n}\sum_{i=1}^{n} \ell\left(y_i w^T x_i\right) + \lambda \|w\|^2 \right) \\
&= \frac{1}{n}\sum_{i=1}^{n} \nabla_w \ell\left(y_i w^T x_i\right) + 2\lambda w
\end{aligned}$$

"Gradient" of SVM Objective

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

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

- By chain rule, we have

$$\begin{aligned} \nabla_w \ell\left(y_i w^T x_i\right) &= \ell'\left(y_i w^T x_i\right) y_i x_i \\ &= \begin{cases} 0 & y_i w^T x_i > 1 \\ -y_i x_i & y_i w^T x_i < 1 \\ \text{undefined} & y_i w^T x_i = 1 \end{cases} \end{aligned}$$

"Gradient" of SVM Objective

$$\nabla_w \ell\left(y_i w^T x_i\right) = \begin{cases} 0 & y_i w^T x_i > 1 \\ -y_i x_i & y_i w^T x_i < 1 \\ \text{undefined} & y_i w^T x_i = 1 \end{cases}$$

So

$$\begin{aligned} \nabla_w J(w) &= \nabla_w \left(\frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i w^T x_i\right) + \lambda \|w\|^2 \right) \\ &= \frac{1}{n} \sum_{i=1}^{n} \nabla_w \ell\left(y_i w^T x_i\right) + 2\lambda w \\ &= \begin{cases} \frac{1}{n} \sum_{i: y_i w^T x_i < 1} \left(-y_i x_i\right) + 2\lambda w & \text{all } y_i w^T x_i \neq 1 \\ \text{undefined} & \text{otherwise} \end{cases} \end{aligned}$$

Gradient Descent on SVM Objective?

- The gradient of the SVM objective is

$$\nabla_w J(w) = \frac{1}{n} \sum_{i: y_i w^T x_i < 1} (-y_i x_i) + 2\lambda w$$

when $y_i w^T x_i \neq 1$ for all i, and otherwise is undefined.

Potential arguments for why we shouldn't care about the points of nondifferentiability:

- If we start with a random w, will we ever hit exactly $y_i w^T x_i = 1$?
- If we did, could we perturb the step size by ε to miss such a point?
- Does it even make sense to check $y_i w^T x_i = 1$ with floating point numbers?

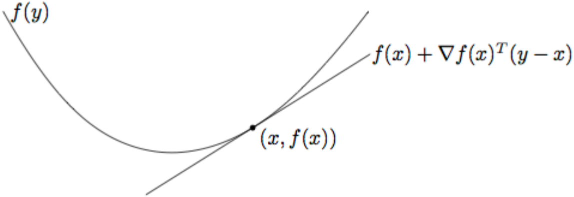
Subgradient

First-Order Condition for Convex, Differentiable Function

- Suppose $f : \mathbb{R}^d \to \mathbb{R}$ is convex and differentiable Then for any $x, y \in \mathbb{R}^d$

$$f(y) \geqslant f(x) + \nabla f(x)^T (y - x)$$

- The linear approximation to f at x is a global underestimator of f:



- This implies that if $\nabla f(x) = 0$ then x is a global minimizer of f.

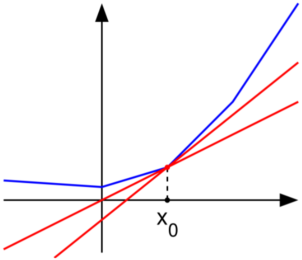
Figure from Boyd & Vandenberghe Fig. 3.2; Proof in Section 3.1.3

Subgradients

Definition

A vector $g \in \mathbb{R}^d$ is a **subgradient** of a *convex* function $f : \mathbb{R}^d \to \mathbb{R}$ at x if for all z,

$$f(z) \geqslant f(x) + g^T(z - x).$$



Blue is a graph of $f(x)$.
Each red line $x \mapsto f(x_0) + g^T(x - x_0)$ is a global lower bound on $f(x)$.

Properties

Definitions

- The set of all subgradients at x is called the **subdifferential**: $\partial f(x)$
- f is **subdifferentiable** at x if $\exists$ at least one subgradient at x.

For convex functions:

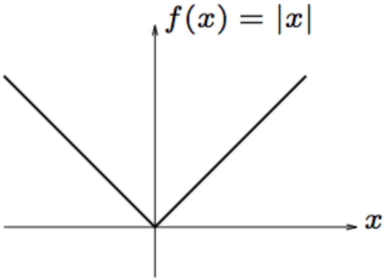
- f is differentiable at x iff $\partial f(x) = \{\nabla f(x)\}$.
- Subdifferential is always non-empty ($\partial f(x) = \emptyset \implies f$ is not convex)
- x is the global optimum iff $0 \in \partial f(x)$.

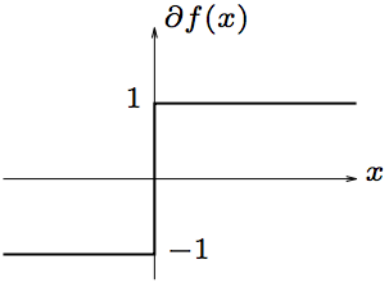
For non-convex functions:

- The subdifferential may be an empty set (no global underestimator).

Subdifferential of Absolute Value

- Consider $f(x) = |x|$





- Plot on right shows $\{(x, g) \mid x \in \mathbb{R},\ g \in \partial f(x)\}$

Boyd EE364b: Subgradients Slides

Subgradient Descent

- Move along the negative subgradient:

$$x^{t+1} = x^t - \eta g \quad \text{where } g \in \partial f(x^t) \text{ and } \eta > 0$$

- This can increase the objective but gets us closer to the minimizer if f is convex and η is small enough:

$$\|x^{t+1} - x^*\| < \|x^t - x^*\|$$

- Subgradients don't necessarily converge to zero as we get closer to x^*, so we need decreasing step sizes.
- Subgradient methods are slower than gradient descent.

Subgradient descent for SVM

SVM objective function:

$$J(w) = \frac{1}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i w^T x_i\right) + \lambda \|w\|^2.$$

Pegasos: stochastic subgradient descent with step size $\eta_t = 1/(t\lambda)$

Input: $\lambda > 0$. Choose $w_1 = 0, t = 0$
While termination condition not met
  For $j = 1, \ldots, n$ (assumes data is randomly permuted)
    $t = t + 1$
    $\eta_t = 1/(t\lambda)$;
    If $y_j w_t^T x_j < 1$
      $w_{t+1} = (1 - \eta_t \lambda) w_t + \eta_t y_j x_j$
    Else
      $w_{t+1} = (1 - \eta_t \lambda) w_t$

Summary

- Subgradient: generalize gradient for non-differentiable convex functions
- Subgradient "descent":
  - General method for non-smooth functions
  - Simple to implement
  - Slow to converge

The Dual Problem

- In addition to subgradient descent, we can directly solve the optimization problem using a Quadratic Programming (QP) solver.
- For convex optimization problem, we can also look into its **dual problem**.

SVM as a Quadratic Program

- The SVM optimization problem is equivalent to

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

- Differentiable objective function
- $n + d + 1$ unknowns and $2n$ affine constraints.
- A **quadratic program** that can be solved by any off-the-shelf QP solver.
- Let's get more insights by examining the dual.

The Lagrangian

The general [inequality-constrained] optimization problem is:

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leqslant 0, \quad i = 1, \ldots, m \end{array}$$

Definition

The **Lagrangian** for this optimization problem is

$$L(x, \lambda) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x).$$

- λ_i's are called **Lagrange multipliers** (also called the **dual variables**).
- Weighted sum of the objective and constraint functions
- Hard constraints $\rightarrow$ soft penalty (objective function)

Lagrange Dual Function

Definition

The **Lagrange dual function** is

$$g(\lambda) = \inf_x L(x, \lambda) = \inf_x \left(f_0(x) + \sum_{i=1}^m \lambda_i f_i(x) \right)$$

- $g(\lambda)$ is concave
- **Lower bound property**: if $\lambda \succeq 0$, $g(\lambda) \leqslant p^*$ where p^* is the optimal value of the optimization problem.
- $g(\lambda)$ can be $-\infty$ (uninformative lower bound)

The Primal and the Dual

- For any **primal form** optimization problem,

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leqslant 0, \;\; i = 1, \ldots, m, \end{array}$$

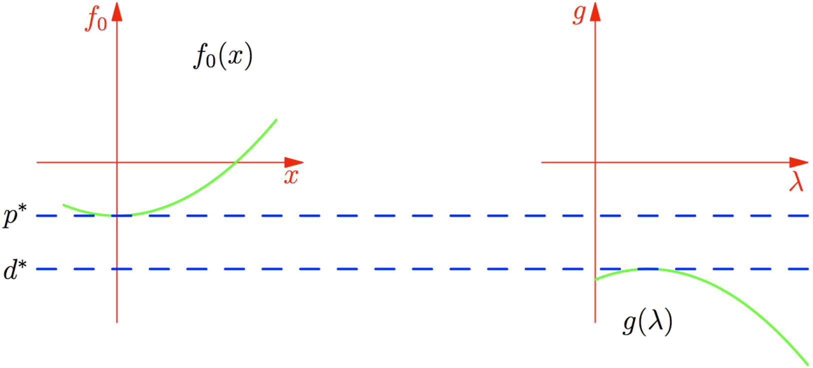
there is a recipe for constructing a corresponding **Lagrangian dual problem:**

$$\begin{array}{ll} \text{maximize} & g(\lambda) \\ \text{subject to} & \lambda_i \geqslant 0, \;\; i = 1, \ldots, m, \end{array}$$

- The dual problem is always a convex optimization problem.

Weak Duality

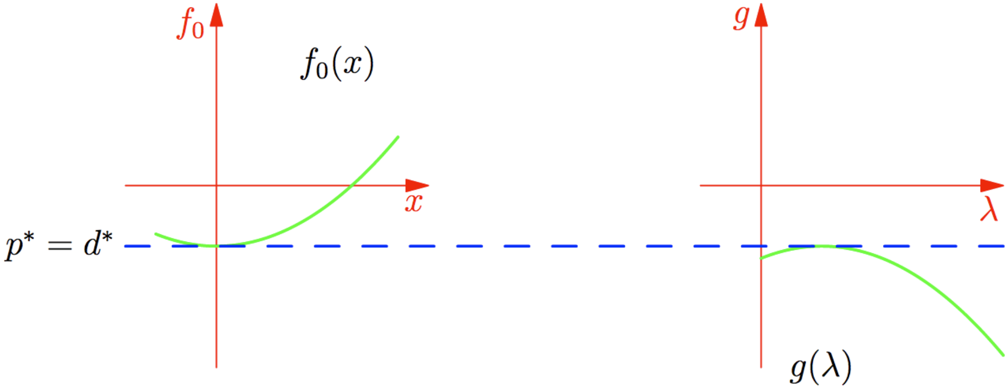
We always have **weak duality:** $p^* \geqslant d^*$.



Plot courtesy of Brett Bernstein.

Strong Duality

For some problems, we have **strong duality**: $p^* = d^*$.



For convex problems, strong duality is fairly typical.

Plot courtesy of Brett Bernstein.

Complementary Slackness

- Assume strong duality. Let x^* be primal optimal and λ^* be dual optimal. Then:

$$\begin{aligned} f_0(x^*) &= g(\lambda^*) = \inf_x L(x, \lambda^*) \quad \text{(strong duality and definition)} \\ &\leqslant L(x^*, \lambda^*) \\ &= f_0(x^*) + \sum_{i=1}^m \lambda_i^* f_i(x^*) \\ &\leqslant f_0(x^*). \end{aligned}$$

Each term in sum $\sum_{i=1} \lambda_i^* f_i(x^*)$ must actually be 0. That is

$$\lambda_i > 0 \implies f_i(x^*) = 0 \quad \text{and} \quad f_i(x^*) < 0 \implies \lambda_i = 0 \quad \forall i$$

This condition is known as **complementary slackness**.

The SVM Dual Problem

SVM Lagrange Multipliers

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

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

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

Strong Duality by Slater's Constraint Qualification

The SVM optimization problem:

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

Slater's constraint qualification:

- Convex problem + affine constraints $\Longrightarrow$ strong duality iff problem is feasible
- Do we have a feasible point?
- For SVM, we have strong duality.

SVM Dual Function: First Order Conditions

Lagrange dual function is the inf over primal variables of L:

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

$$\partial_w L = 0$$

$$\partial_b L = 0$$

$$\partial_{\xi_i} L = 0$$

SVM Dual Function

- Substituting these conditions back into L, the second term disappears.
- First and third terms become

- Putting it together, the dual function is

SVM Dual Problem

- The **dual function** is

$$g(\alpha,\lambda) = \begin{cases} \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j=1}^n \alpha_i\alpha_j y_i y_j x_j^T x_i & \substack{\sum_{i=1}^n \alpha_i y_i = 0 \\ \alpha_i + \lambda_i = \frac{c}{n},\ \text{all } i} \\ -\infty & \text{otherwise.} \end{cases}$$

- The **dual problem** is $\sup_{\alpha,\lambda \succeq 0} g(\alpha,\lambda)$:

$$\begin{array}{ll} \sup_{\alpha,\lambda} & \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j=1}^n \alpha_i\alpha_j y_i y_j x_j^T x_i \\ \text{s.t.} & \sum_{i=1}^n \alpha_i y_i = 0 \\ & \alpha_i + \lambda_i = \frac{c}{n} \quad \alpha_i, \lambda_i \geqslant 0,\ i = 1,\ldots,n \end{array}$$

Insights from the Dual Problem

KKT Conditions

For convex problems, if Slater's condition is satisfied, then **KKT conditions** provide necessary and sufficient conditions for the optimal solution.

- Primal feasibility: $f_i(x) \leqslant 0 \quad \forall i$
- Dual feasibility: $\lambda \succeq 0$
- Complementary slackness: $\lambda_i f_i(x) = 0$
- First-order condition:

$$\frac{\partial}{\partial x} L(x, \lambda) = 0$$

The SVM Dual Solution

- We found the SVM dual problem can be written as:

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

- Given solution α^* to dual, primal solution is $w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i$.
- The solution is in the space spanned by the inputs.
- Note $\alpha_i^* \in [0, \frac{c}{n}]$. So c controls max weight on each example. (**Robustness**!)
  - What's the relation between c and regularization?

Complementary Slackness Conditions

- Recall our primal constraints and Lagrange multipliers:

Lagrange Multiplier	Constraint
λ_i	$-\xi_i \leqslant 0$
α_i	$(1 - y_i f(x_i)) - \xi_i \leqslant 0$

- Recall first order condition $\nabla_{\xi_i} L = 0$ gave us $\lambda_i^* = \frac{c}{n} - \alpha_i^*$.

- By strong duality, we must have **complementary slackness**:

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

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

Consequences of Complementary Slackness

By strong duality, we must have **complementary slackness**.

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

Recall "**slack variable**" $\xi_i^* = \max(0, 1-y_i f^*(x_i))$ is the hinge loss on (x_i, y_i).

- If $y_i f^*(x_i) > 1$ then the margin loss is $\xi_i^* = 0$, and we get $\alpha_i^* = 0$.
- If $y_i f^*(x_i) < 1$ then the margin loss is $\xi_i^* > 0$, so $\alpha_i^* = \frac{c}{n}$.
- If $\alpha_i^* = 0$, then $\xi_i^* = 0$, which implies no loss, so $y_i f^*(x) \geqslant 1$.
- If $\alpha_i^* \in \left(0, \frac{c}{n}\right)$, then $\xi_i^* = 0$, which implies $1 - y_i f^*(x_i) = 0$.

Complementary Slackness Results: Summary

If α^* is a solution to the dual problem, then primal solution is

$$w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i \quad \text{where} \alpha_i^* \in [0, \frac{c}{n}].$$

Relation between margin and example weights (α_i's):

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

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

Support Vectors

- If α^* is a solution to the dual problem, then primal solution is

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

  with $\alpha_i^* \in [0, \frac{c}{n}]$.

- The x_i's corresponding to $\alpha_i^* > 0$ are called **support vectors.**
- Few margin errors or "on the margin" examples $\Longrightarrow$ sparsity in input examples.

Dual Problem: Dependence on x through inner products

- SVM Dual Problem:

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

- Note that all dependence on inputs x_i and x_j is through their inner product: $\langle x_j, x_i \rangle = x_j^T x_i$.
- We can replace $x_j^T x_i$ by other products...
- This is a "kernelized" objective function.

Feature Maps

The Input Space $\mathcal{X}$

- Our general learning theory setup: no assumptions about $\mathcal{X}$
- But $\mathcal{X} = \mathbf{R}^d$ for the specific methods we've developed:
  - Ridge regression
  - Lasso regression
  - Support Vector Machines
- Our hypothesis space for these was all affine functions on $\mathbf{R}^d$:

$$\mathcal{F} = \left\{ x \mapsto w^T x + b \mid w \in \mathbf{R}^d, b \in \mathbf{R} \right\}.$$

- What if we want to do prediction on inputs not natively in $\mathbf{R}^d$?

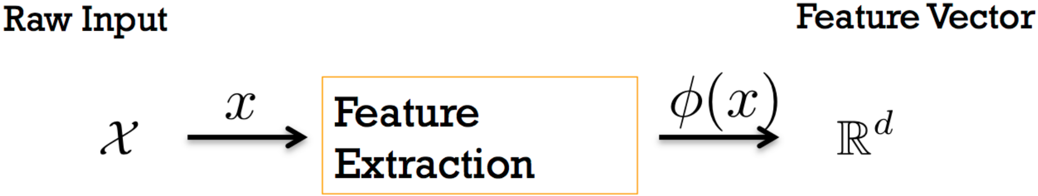
The Input Space $\mathcal{X}$

- Often want to use inputs not natively in $\mathbb{R}^d$:
  - Text documents
  - Image files
  - Sound recordings
  - DNA sequences
- They may be represented in numbers, but...
- The *i*th entry of each sequence should have the same "meaning"
- All the sequences should have the same length

Feature Extraction

Definition

Mapping an input from $\mathcal{X}$ to a vector in $\mathbb{R}^d$ is called **feature extraction** or **featurization**.



Linear Models with Explicit Feature Map

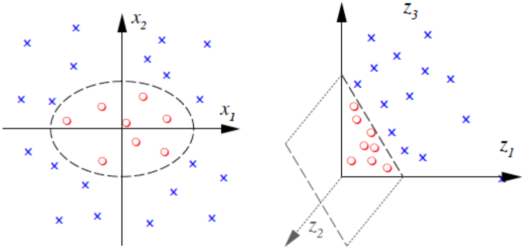
- Input space: $\mathcal{X}$ (no assumptions)
- Introduce **feature map** $\phi : \mathcal{X} \to \mathrm{R}^d$
- The feature map maps into the **feature space** R^d.
- Hypothesis space of affine functions on feature space:

$$\mathcal{F} = \left\{ x \mapsto w^T \phi(x) + b \mid w \in \mathrm{R}^d, b \in \mathrm{R} \right\}.$$

Geometric Example: Two class problem, nonlinear boundary

$$\Phi : R^2 \rightarrow R^3$$

$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt(2) x_1 x_2, x_2^2)$$



- With identity feature map $\phi(x) = (x_1, x_2)$ and linear models, can't separate regions
- With appropriate featurization $\phi(x) = \left(x_1, x_2, x_1^2 + x_2^2\right)$, becomes linearly separable .
- Video: http://youtu.be/3liCbRZPrZA

Expressivity of Hypothesis Space

- For linear models, to grow the hypothesis spaces, we must add features.
- Sometimes we say a larger hypothesis is more expressive.
  - (can fit more relationships between input and action)
- Many ways to create new features.

Handling Nonlinearity with Linear Methods

Example Task: Predicting Health

- General Philosophy: Extract every feature that might be relevant
- Features for medical diagnosis
  - height
  - weight
  - body temperature
  - blood pressure
  - etc...

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

Feature Issues for Linear Predictors

- For linear predictors, it's important **how** features are added
  - The relation between a feature and the label may not be linear
  - There may be complex dependence among features
- Three types of nonlinearities can cause problems:
  - Non-monotonicity
  - Saturation
  - Interactions between features

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

Non-monotonicity: The Issue

- Feature Map: $\phi(x) = [1, \text{temperature}(x)]$
- Action: Predict health score $y \in R$ (positive is good)
- Hypothesis Space $\mathcal{F}$={affine functions of temperature}
- Issue:
  - Health is not an affine function of temperature.
  - Affine function can either say
    - Very high is bad and very low is good, or
    - Very low is bad and very high is good,
    - But here, both extremes are bad.

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Non-monotonicity: Solution 1

- Transform the input:

$$\phi(x) = \left[1, \{\text{temperature(x)-37}\}^2\right],$$

  where 37 is “normal” temperature in Celsius.

- Ok, but requires manually-specified domain knowledge
  - Do we really need that?
  - What does $w^T\phi(x)$ look like?

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Non-monotonicity: Solution 2

- Think less, put in more:

$$\phi(x) = \left[1, \text{temperature}(x), \{\text{temperature}(x)\}^2\right].$$

- More expressive than Solution 1.

General Rule

Features should be simple building blocks that can be pieced together.

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Saturation: The Issue

- Setting: Find products relevant to user's query
- Input: Product x
- Output: Score the relevance of x to user's query
- Feature Map:

$$\phi(x) = [1, N(x)],$$

  where $N(x) =$ number of people who bought x.
- We expect a monotonic relationship between $N(x)$ and relevance, but also expect diminishing return.

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Saturation: Solve with nonlinear transform

- Smooth nonlinear transformation:

$$\phi(x) = [1, \log\{1 + N(x)\}]$$

  - $\log(\cdot)$ good for values with large dynamic ranges

- Discretization (a discontinuous transformation):

$$\phi(x) = (\mathbb{1}[0 \leqslant N(x) < 10], \mathbb{1}[10 \leqslant N(x) < 100], \ldots)$$

  - Small buckets allow quite flexible relationship

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Interactions: The Issue

- Input: Patient information x
- Action: Health score $y \in R$ (higher is better)
- Feature Map

$$\phi(x) = [\text{height}(x), \text{weight}(x)]$$

- Issue: It's the weight *relative* to the height that's important.
- Impossible to get with these features and a linear classifier.
- Need some **interaction** between height and weight.

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Interactions: Approach 1

- Google "ideal weight from height"
- J. D. Robinson's "ideal weight" formula:

$$\text{weight(kg)} = 52 + 1.9\,[\text{height(in)} - 60]$$

- Make score square deviation between height(h) and ideal weight(w)

$$f(x) = (52 + 1.9\,[h(x) - 60] - w(x))^2$$

- WolframAlpha for complicated Mathematics:

$$f(x) = 3.61h(x)^2 - 3.8h(x)w(x) - 235.6h(x) + w(x)^2 + 124w(x) + 3844$$

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Interactions: Approach 2

- Just include all second order features:

$$\phi(x) = \left[1, h(x), w(x), h(x)^2, w(x)^2, \underbrace{h(x)w(x)}_{\text{cross term}}\right]$$

- More flexible, no Google, no WolframAlpha.

General Principle

Simpler building blocks replace a single "smart" feature.

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Monomial Interaction Terms

Interaction terms are useful building blocks to model non-linearities in features.

- Suppose we start with $x = (1, x_1, \ldots, x_d) \in \mathrm{R}^{d+1} = \mathcal{X}$.
- Consider adding all **monomials** of degree M: $x_1^{p_1} \cdots x_d^{p_d}$, with $p_1 + \cdots + p_d = M$.
  - Monomials with degree 2 in 2D space: x_1^2, x_2^2, $x_1 x_2$

Big Feature Spaces

This leads to extremely large data matrices

- For $d = 40$ and $M = 8$, we get 314457495 features.

Very large feature spaces have two potential issues:

- Overfitting
- Memory and computational costs

Solutions:

- Overfitting we handle with regularization.
- **Kernel methods** can help with memory and computational costs when we go to high (or infinite) dimensional spaces.