SVM and Kernel Methods

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SVM as an Optimization Problem

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

- The first term is the L2 regularizer.
- The second term is the Hinge loss (slack variables).

Subgradient Descent

Now that we have the objective, can we do SGD on it?

Subgradient: generalize gradient for non-differentiable convex functions

SVM Optimization Problem (no intercept)

- 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?

However, would gradient descent work if the objective is not differentiable?

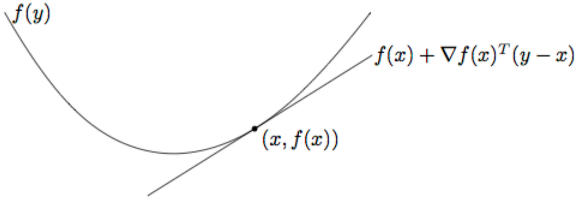
Subgradient

First-Order Condition for Convex, Differentiable Function

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

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

- 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.

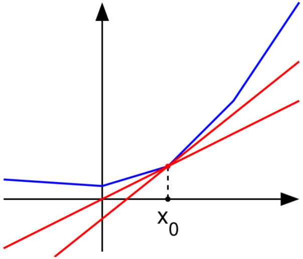
Figure from Boyd & Vandenberghe Fig. 3.2; Proof in Section 3.1.3

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:

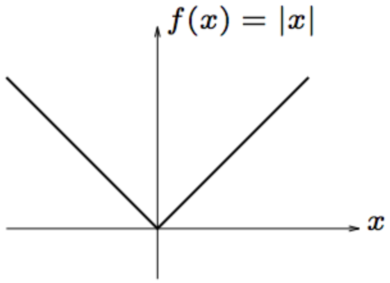
- f is differentiable at x iff $\partial f(x) = \{\nabla f(x)\}$.
- Subdifferential is always non-empty ($\partial f(x) = \emptyset \implies f$ is not convex)
- x is the global optimum iff $0 \in \partial f(x)$.

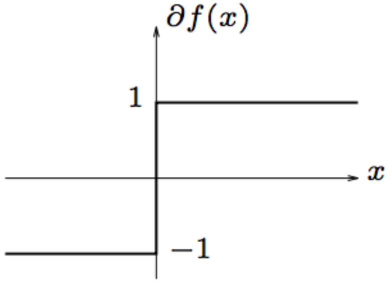
For non-convex functions:

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

Subdifferential of Absolute Value

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



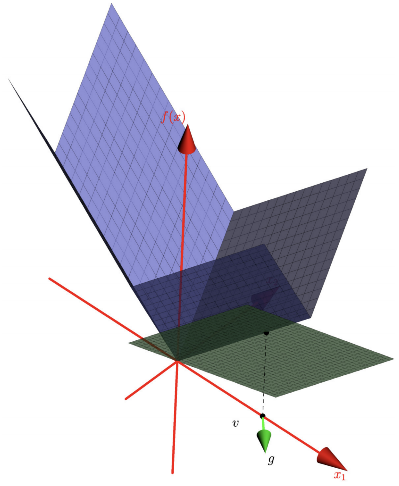


- Plot on right shows $\{(x, g) \mid x \in \mathbb{R},\ g \in \partial f(x)\}$

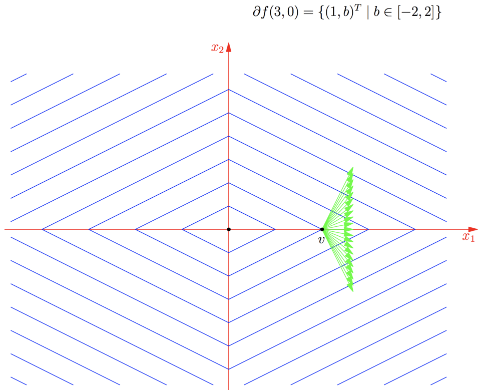
Boyd EE364b: Subgradients Slides

Subgradients of $f(x_1, x_2) = |x_1| + 2|x_2|$

- Let's find the subdifferential of $f(x_1, x_2) = |x_1| + 2|x_2|$ at $(3, 0)$.
- First coordinate of subgradient must be 1, from $|x_1|$ part (at $x_1 = 3$).
- Second coordinate of subgradient can be anything in $[-2, 2]$.
- So graph of $h(x_1, x_2) = f(3, 0) + g^T(x_1 - 3, x_2 - 0)$ is a global underestimate of $f(x_1, x_2)$, for any $g = (g_1, g_2)$, where $g_1 = 1$ and $g_2 \in [-2, 2]$.



Subdifferential on Contour Plot



Contour plot of $f(x_1,x_2) = |x_1| + 2|x_2|$, with set of subgradients at $(3,0)$. .

Plot courtesy of Brett Bernstein.

Basic Rules for Calculating Subdifferential

- Non-negative scaling: $\partial \alpha f(x) = \alpha \partial f(x)$ for $(\alpha > 0)$
- Summation: $\partial(f_1(x) + f_2(x)) = d_1 + d_2$ for any $d_1 \in \partial f_1$ and $d_2 \in \partial f_2$
- Composing with affine functions: $\partial f(Ax+b) = A^T \partial f(z)$ where $z = Ax+b$
- max: convex combinations of argmax gradients

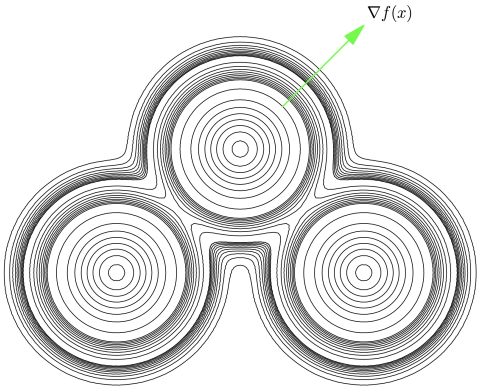
$$\partial \max(f_1(x), f_2(x)) = \begin{cases} \nabla f_1(x) & \text{if } f_1(x) > f_2(x), \\ \nabla f_2(x) & \text{if } f_1(x) < f_2(x), \\ \nabla \theta f_1(x) + (1-\theta) f_2(x) & \text{if } f_1(x) = f_2(x), \end{cases}$$

where $\theta \in [0,1]$.

Subgradient Descent

Gradient orthogonal to level sets

We know that gradient points to the fastest ascent direction. What about subgradients?



Plot courtesy of Brett Bernstein.

Contour Lines and Subgradients

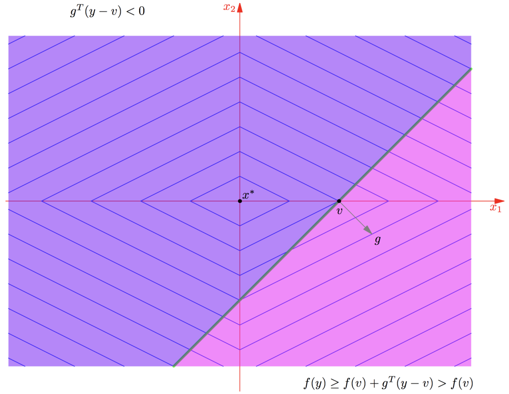
A hyperplane H **supports** a set S if H intersects S and all of S lies one one side of H.

Claim: If $f : \mathbf{R}^d \to \mathbf{R}$ has subgradient g at x_0, then the hyperplane H orthogonal to g at x_0 must **support** the level set $S = \left\{x \in \mathbf{R}^d \mid f(x) = f(x_0)\right\}$.

Proof:

- For any y, we have $f(y) \geqslant f(x_0) + g^T(y - x_0)$. (def of subgradient)
- If y is strictly on side of H that g points in,
  - then $g^T(y - x_0) > 0$.
  - So $f(y) > f(x_0)$.
  - So y is not in the level set S.
- $\therefore$ All elements of S must be on H or on the $-g$ side of H.

Subgradient of $f(x_1, x_2) = |x_1| + 2|x_2|$



- Points on g side of H have larger f-values than $f(x_0)$. (from proof)
- But points on $-g$ side may **not** have smaller f-values.
- So $-g$ may **not** be a descent direction. (shown in figure)

Plot courtesy of Brett Bernstein.

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:

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

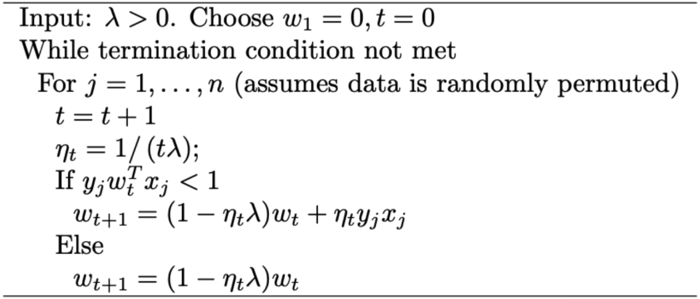
- Subgradients don't necessarily converge to zero as we get closer to x^*, so we need decreasing step sizes.
- Subgradient methods are slower than gradient descent.

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 QP solver.

Let's study its dual problem to gain addition insights (which will be useful for next week!)

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 learn more 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 constraints (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,

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

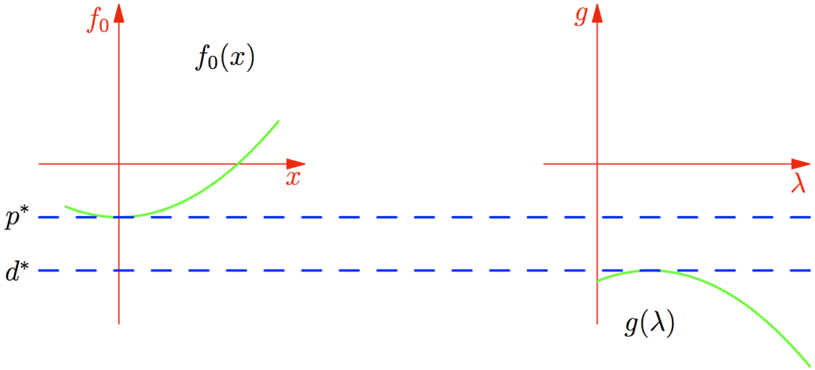
  there is a recipe for constructing a corresponding **Lagrangian dual problem:**

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

- The dual problem is always a convex optimization problem.
- The dual variables often have interesting and relevant interpretations.
- The dual variables provide certificates for optimality.

Weak Duality

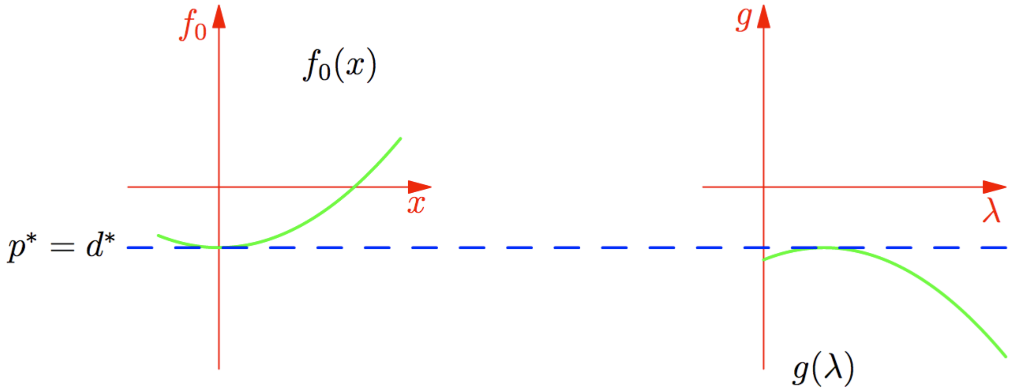
We always have **weak duality:** $p^* \geqslant d^*$.



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

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

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

Strong Duality by Slater's Constraint Qualification

The SVM optimization problem:

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

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:

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

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

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

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

SVM Dual Function

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

$$
\begin{aligned}
\frac{1}{2}w^Tw &= \frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^T x_j \\
\sum_{i=1}^{n}\alpha_i\left(1-y_i\left[w^Tx_i+b\right]\right) &= \sum_{i=1}^{n}\alpha_i-\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j x_j^T x_i - b\underbrace{\sum_{i=1}^{n}\alpha_i y_i}_{=0}.
\end{aligned}
$$

- Putting it together, the dual function is

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

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):

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

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

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 $\implies$ sparsity in input examples.

Teaser for Kernelization

Dual Problem: Dependence on x through inner products

- SVM Dual Problem:

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

- 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 $\mathcal{X} = \mathrm{R}^d$ for the specific methods we've developed:
    - Ridge regression
    - Lasso regression
    - Support Vector Machines
- Our hypothesis space for these was all affine functions on R^d:

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

- What if we want to do prediction on inputs not natively in R^d?

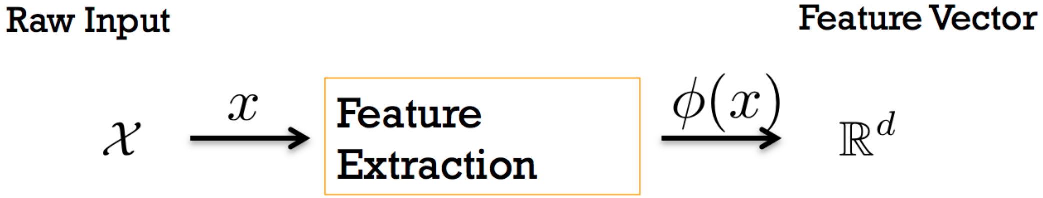
The Input Space $\mathcal{X}$

- Often want to use inputs not natively in R^d:
  - Text documents
  - Image files
  - Sound recordings
  - DNA sequences
- But everything in a computer is a sequence of numbers
  - The ith 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 R^d is called **feature extraction** or **featurization**.



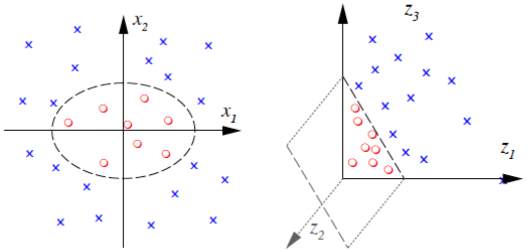
Linear Models with Explicit Feature Map

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

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

Geometric Example: Two class problem, nonlinear boundary

$$\Phi : R^2 \to R^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{(}2)x_1x_2, x_2^2)$$



- 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 $y \in \mathbb{R}$ (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.

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

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?

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

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.

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

Saturation: The Issue

- Setting: Find products relevant to user's query
- Input: Product x
- Action: 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.

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

Saturation: Solve with nonlinear transform

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.

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

Interactions: Approach 1

- Google "ideal weight from height"
- J. D. Robinson's "ideal weight" formula (for a male):

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

- 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:

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

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

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.

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

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, $x_1 x_2$
- How many features will we end up with? $\binom{M+d-1}{M}$ ("stars and bars")
- This leads to extremely large data matrices
  - For $d = 40$ and $M = 8$, we get 314457495 features.

Big Feature Spaces

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.

The Kernel Trick

SVM with Explicit Feature Map

- Let $\psi : \mathcal{X} \to \mathbf{R}^d$ be a feature map.
- The SVM objective (with explicit feature map):

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

- Computation is costly if d is large (e.g. with high-degree monomials)
- Last time we mentioned an equivalent optimization problem from Lagrangian duality.

SVM Dual Problem

- By Lagrangian duality, it is equivalent to solve the following dual problem:

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

- If α^* is an optimal value, then

$$w^* = \sum_{i=1}^{n} \alpha_i^* y_i \psi(x_i) \quad \text{and} \quad \hat{f}(x) = \sum_{i=1}^{n} \alpha_i^* y_i \psi(x_i)^T \psi(x).$$

- Key observation: $\psi(x)$ only shows up in inner products with another $\psi(x')$ *for both training and inference*.

Compute the Inner Products

Consider 2D data. Let's introduce degree-2 monomials using $\psi : \mathrm{R}^2 \to \mathrm{R}^3$.

$$(x_1, x_2) \mapsto (x_1^2, \sqrt{2}x_1x_2, x_2^2).$$

The inner product is

$$\begin{aligned}
\psi(x)^T\psi(x') &= x_1^2 x_1'^2 + (\sqrt{2}x_1x_2)(\sqrt{2}x_1'x_2') + x_2^2 x_2'^2 \\
&= (x_1x_1')^2 + 2(x_1x_1')(x_2x_2') + (x_2x_2')^2 \\
&= (x_1x_1' + x_2x_2')^2 \\
&= (x^Tx')^2
\end{aligned}$$

We can calculate the inner product $\psi(x)^T\psi(x')$ in the original input space without accessing the features $\psi(x)$!

Compute the Inner Products

Now, consider monomials up to degree-2:

$$(x_1, x_2) \mapsto (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2).$$

The inner product can be computed by

$$\psi(x)^T\psi(x') = (1 + x^Tx')^2 \quad \text{(check)}.$$

More generally, for features maps producing monomials up to degree-p, we have

$$\psi(x)^T\psi(x') = (1 + x^Tx')^p.$$

(Note that the coefficients of each monomial in ψ may not be 1)

Kernel trick: we do not need explicit features to calculate inner products.

- Using explicit features: $O(d^p)$
- Using implicit computation: $O(d)$

Kernel Function

The Kernel Function

- **Input space**: $\mathcal{X}$
- **Feature space**: $\mathcal{H}$ (a Hilbert space, e.g. $\mathbf{R}^d$)
- **Feature map**: $\psi : \mathcal{X} \to \mathcal{H}$
- The **kernel function** corresponding to ψ is

$$k(x, x') = \langle \psi(x), \psi(x') \rangle ,$$

  where $\langle \cdot, \cdot \rangle$ is the inner product associated with $\mathcal{H}$.

Why introduce this new notation $k(x, x')$?

- We can often evaluate $k(x, x')$ without explicitly computing $\psi(x)$ and $\psi(x')$.

When can we use the kernel trick?

Some Methods Can Be "Kernelized"

Definition

A method is **kernelized** if every feature vector $\psi(x)$ only appears inside an inner product with another feature vector $\psi(x')$. This applies to both the optimization problem and the prediction function.

The SVM Dual is a kernelization of the original SVM formulation.

Optimization:

$$\begin{array}{rl} \text{maximize} & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \psi(x_j)^T \psi(x_i) \\ \text{s.t.} & \sum_{i=1}^{n} \alpha_i y_i = 0 \quad \text{and} \quad \alpha_i \in \left[0, \frac{c}{n}\right] \quad \forall i. \end{array}$$

Prediction:

$$\hat{f}(x) = \sum_{i=1}^{n} \alpha_i^* y_i \psi(x_i)^T \psi(x).$$

The Kernel Matrix

Definition

The **kernel matrix** for a kernel k on $x_1, \dots, x_n \in \mathcal{X}$ is

$$K = \left(k(x_i, x_j)\right)_{i,j} = \begin{pmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & \ddots & \dots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{pmatrix} \in \mathrm{R}^{n \times n}.$$

- In ML this is also called a **Gram matrix**, but traditionally (in linear algebra), Gram matrices are defined without reference to a kernel or feature map.

The Kernel Matrix

- The kernel matrix summarizes all the information we need about the training inputs $x_1, \ldots, x_n$ to solve a kernelized optimization problem.
- In the kernelized SVM, we can replace $\psi(x_i)^T \psi(x_j)$ with K_{ij}:

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

Kernel Methods

Given a kernelized ML algorithm (i.e. all $\psi(x)$'s show up as $\langle\psi(x),\psi(x')\rangle$),

- Can swap out the inner product for a new kernel function.
- New kernel may correspond to a very high-dimensional feature space.
- Once the kernel matrix is computed, the computational cost depends on number of data points n, rather than the dimension of feature space d.
- Useful when $d >> n$.
- Computing the kernel matrix may still depend on d and the essence of the **trick** is getting around this $O(d)$ dependence.

Example Kernels

Kernels as Similarity Scores

- Often useful to think of the $k(x, x')$ as a **similarity score** for x and x'.
- We can design similarity functions without thinking about the explicit feature map, e.g. "string kernels", "graph kerners".
- How do we know that our kernel functions actually correspond to inner products in some feature space?

How to Get Kernels?

- Explicitly construct $\psi(x) : \mathcal{X} \to \mathbf{R}^d$ (e.g. monomials) and define $k(x, x') = \psi(x)^T \psi(x')$.
- Directly define the kernel function $k(x, x')$ ("similarity score"), and verify it corresponds to $\langle \psi(x), \psi(x') \rangle$ for some ψ.

There are many theorems to help us with the second approach.

Linear Algebra Review: Positive Semidefinite Matrices

Definition

A real, symmetric matrix $M \in \mathbb{R}^{n \times n}$ is **positive semidefinite (psd)** if for any $x \in \mathbb{R}^n$,

$$x^T M x \geqslant 0.$$

Theorem

The following conditions are each necessary and sufficient for a symmetric matrix M to be positive semidefinite:

- *M can be factorized as $M = R^T R$, for some matrix R.*
- *All eigenvalues of M are greater than or equal to 0.*

Positive Definite Kernel

Definition

A symmetric function $k : \mathcal{X} \times \mathcal{X} \to R$ is a **positive definite (pd)** kernel on $\mathcal{X}$ if for any finite set $\{x_1, \dots, x_n\} \in \mathcal{X}$ $(n \in \mathbb{N})$, the kernel matrix on this set

$$K = \left(k(x_i, x_j)\right)_{i,j} = \begin{pmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & \ddots & \dots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{pmatrix}$$

is a positive semidefinite matrix.

- Symmetric: $k(x, x') = k(x', x)$
- The kernel matrix needs to be positive semidefinite for any finite set of points.
- Equivalent definition: $\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j k(x_i, x_j) \geqslant 0$ given $\alpha_i \in R\ \forall i$.

Mercer's Theorem

Theorem

A symmetric function $k(x,x')$ can be expressed as an inner product

$$k(x,x') = \langle \psi(x), \psi(x') \rangle$$

for some ψ if and only if $k(x,x')$ is ***positive definite****.*

- Proving a kernel function is positive definite is typically not easy.
- But we can construct new kernels from valid kernels.

Generating New Kernels from Old

- Suppose $k, k_1, k_2 : \mathcal{X} \times \mathcal{X} \to \mathbf{R}$ are pd kernels. Then so are the following:

$$\begin{aligned}
k_{\text{new}}(x,x') &= \alpha k(x,x') \quad \text{for } \alpha \geqslant 0 \quad \text{(non-negative scaling)} \\
k_{\text{new}}(x,x') &= k_1(x,x') + k_2(x,x') \quad \text{(sum)} \\
k_{\text{new}}(x,x') &= k_1(x,x')k_2(x,x') \quad \text{(product)} \\
k_{\text{new}}(x,x') &= k(\psi(x),\psi(x')) \text{ for any function } \psi(\cdot) \quad \text{(recursion)} \\
k_{\text{new}}(x,x') &= f(x)f(x') \text{ for any function } f(\cdot) \quad (f \text{ as 1D feature map})
\end{aligned}$$

- Lots more theorems to help you construct new kernels from old.

Based on Mark Schmidt's slides:https://www.cs.ubc.ca/~schmidtm/Courses/540-W19/L12.5.pdf

Linear Kernel

- Input space: $\mathcal{X} = \mathbf{R}^d$
- Feature space: $\mathcal{H} = \mathbf{R}^d$, with standard inner product
- Feature map
$$\psi(x) = x$$
- Kernel:
$$k(x, x') = x^T x'$$

Quadratic Kernel in $\mathbf{R}^d$

- Input space $\mathcal{X} = \mathbf{R}^d$
- Feature space: $\mathcal{H} = \mathbf{R}^D$, where $D = d + \binom{d}{2} \approx d^2/2$.
- Feature map:

$$\psi(x) = (x_1, \ldots, x_d, x_1^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_ix_j, \ldots \sqrt{2}x_{d-1}x_d)^T$$

- Then for $\forall x, x' \in \mathbf{R}^d$

$$\begin{aligned} k(x,x') &= \langle \psi(x), \psi(x') \rangle \\ &= \langle x, x' \rangle + \langle x, x' \rangle^2 \end{aligned}$$

- Computation for inner product with explicit mapping: $O(d^2)$
- Computation for implicit kernel calculation: $O(d)$.

Polynomial Kernel in $\mathbf{R}^d$

- Input space $\mathcal{X} = \mathbf{R}^d$
- Kernel function:

$$k(x, x') = \left(1 + \langle x, x' \rangle\right)^M$$

- Corresponds to a feature map with all monomials up to degree M.
- For any M, computing the kernel has same computational cost
- Cost of explicit inner product computation grows rapidly in M.

Radial Basis Function (RBF) / Gaussian Kernel

Input space $\mathcal{X} = \mathbf{R}^d$

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

where σ^2 is known as the bandwidth parameter.

- Probably the most common nonlinear kernel.
- Does it act like a similarity score?
- Have we departed from our "inner product of feature vector" recipe?
  - Yes and no: corresponds to an infinite dimensional feature vector

Remaining Questions

Our current recipe:

- Recognize kernelized problem: $\psi(x)$ only occur in inner products $\psi(x)^T\psi(x')$
- Pick a kernel function ("similarity score")
- Compute the kernel matrix (n by n where n is the dataset size)
- Optimize the model and make predictions by accessing the kernel matrix

Next: When can we apply kernelization?

SVM solution is in the "span of the data"

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

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

- Given dual solution α^*, primal solution is $w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i$.
- Notice: w^* is a linear combination of training inputs $x_1, \ldots, x_n$.
- We refer to this phenomenon by saying "w^* is in the **span of the data**."
  - Or in math, $w^* \in \operatorname{span}(x_1, \ldots, x_n)$.

Ridge regression solution is in the "span of the data"

- The ridge regression solution for regularization parameter $\lambda > 0$ is

$$w^* = \underset{w \in \mathbf{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_2^2.$$

- This has a closed form solution (Homework #3):

$$w^* = \left(X^T X + \lambda I \right)^{-1} X^T y,$$

where X is the design matrix, with $x_1, \dots, x_n$ as rows.

Ridge regression solution is in the "span of the data"

- Rearranging $w^* = \left(X^T X + \lambda I\right)^{-1} X^T y$, we can show that (also Homework #3):

$$\begin{aligned} w^* &= X^T \underbrace{\left(\frac{1}{\lambda} y - \frac{1}{\lambda} X w^*\right)}_{\alpha^*} \\ &= X^T \alpha^* = \sum_{i=1}^{n} \alpha_i^* x_i. \end{aligned}$$

- So w^* is in the span of the data.
  - i.e. $w^* \in \operatorname{span}(x_1, \ldots, x_n)$

If solution is in the span of the data, we can reparameterize

- The ridge regression solution for regularization parameter $\lambda > 0$ is

$$w^* = \underset{w \in \mathrm{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_2^2.$$

- We now know that $w^* \in \operatorname{span}(x_1, \ldots, x_n) \subset \mathrm{R}^d$.
- So rather than minimizing over all of R^d, we can minimize over $\operatorname{span}(x_1, \ldots, x_n)$.

$$w^* = \underset{w \in \operatorname{span}(x_1, \ldots, x_n)}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_2^2.$$

- Let's reparameterize the objective by replacing w as a linear combination of the inputs.

If solution is in the span of the data, we can reparameterize

- Note that for any $w \in \operatorname{span}(x_1, \ldots, x_n)$, we have $w = X^T \alpha$, for some $\alpha \in \mathbb{R}^n$.
- So let's replace w with $X^T \alpha$ in our optimization problem:

$$
\begin{aligned}
\text{[original] } w^* &= \underset{w \in \mathbb{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_2^2 \\
\text{[reparameterized] } \alpha^* &= \underset{\alpha \in \mathbb{R}^n}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ \left(X^T \alpha \right)^T x_i - y_i \right\}^2 + \lambda \|X^T \alpha\|_2^2 .
\end{aligned}
$$

- To get w^* from the reparameterized optimization problem, we just take $w^* = X^T \alpha^*$.
- We changed the dimension of our optimization variable from d to n. Is this useful?

Consider very large feature spaces

- Suppose we have a 300-million dimension feature space [very large]
    - (e.g. using high order monomial interaction terms as features, as described last lecture)
- Suppose we have a training set of 300,000 examples [fairly large]
- In the original formulation, we solve a 300-million dimension optimization problem.
- In the reparameterized formulation, we solve a 300,000-dimension optimization problem.
- This is why we care about when the solution is in the span of the data.
- This reparameterization is interesting when we have more features than data ($d \gg n$).

More General

- For SVM and ridge regression, we found that the solution is in the span of the data.
- The Representer Theorem shows that this "span of the data" result occurs far more generally.

The Representer Theorem (Optional)

- **Generalized objective**:

$$w^* = \arg\min_{w \in \mathcal{H}} R\left(\|w\|\right) + L\left(\langle w, x_1\rangle, \ldots, \langle w, x_n\rangle\right)$$

- Representer theorem tells us we can look for w^* in the span of the data:

$$w^* = \arg\min_{w \in \text{span}(x_1, \ldots, x_n)} R\left(\|w\|\right) + L\left(\langle w, x_1\rangle, \ldots, \langle w, x_n\rangle\right).$$

- So we can reparameterize as before:

$$\alpha^* = \arg\min_{\alpha \in \mathbf{R}^n} R\left(\left\|\sum_{i=1}^n \alpha_i x_i\right\|\right) + L\left(\left\langle \sum_{i=1}^n \alpha_i x_i, x_1\right\rangle, \ldots, \left\langle \sum_{i=1}^n \alpha_i x_i, x_n\right\rangle\right).$$

- Our reparameterization trick applies much more broadly than SVM and ridge.

Summary

- We used duality for SVM and bare hands for ridge regression to find their kernelized version.
- Many other algorithms can be kernelized.
- Our principled tool for kernelization is reparameterization by the representer theorem.
- Representer theorem says that all norm-regularized linear models can be kernelized.
- Once kernelized, we can apply the kernel trick: doesn't need to represent $\phi(x)$ explicitly.