SVM and Kernel Methods

Mengye Ren

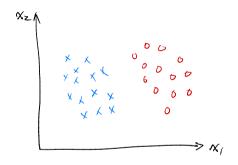
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Maximum Margin Classifier

Linearly Separable Data

Consider a linearly separable dataset \mathfrak{D} :



Find a separating hyperplane such that

- $w^T x_i > 0$ for all x_i where $y_i = +1$
- $w^T x_i < 0$ for all x_i where $y_i = -1$

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The Perceptron Algorithm

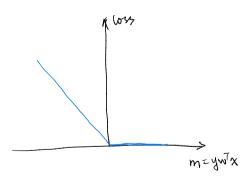
- Initialize $w \leftarrow 0$
- While not converged (exists misclassified examples)
 - For $(x_i, y_i) \in \mathcal{D}$
 - If $y_i w^T x_i < 0$ (wrong prediction)
 - Update $w \leftarrow w + y_i x_i$
- Intuition: move towards misclassified positive examples and away from negative examples
- Guarantees to find a zero-error classifier (if one exists) in finite steps
- What is the loss function if we consider this as a SGD algorithm?

Minimize the Hinge Loss

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Perceptron Loss

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

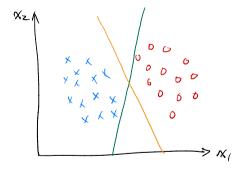


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Maximum-Margin Separating Hyperplane

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

Which one do we pick?

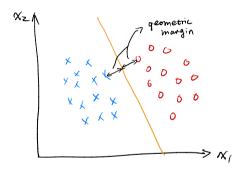


(Perceptron does not return a unique solution.)

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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

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

Definition (geometric margin)

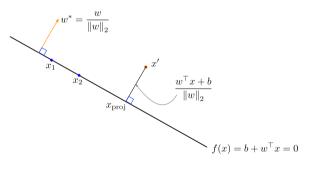
Let H be a hyperplane that separates the data (x_i, y_i) for i = 1, ..., n. The **geometric margin** of this hyperplane is

$$\min_{i} d(x_i, H),$$

the distance from the hyperplane to the closest data point.

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Distance between a Point and a Hyperplane



- Any point on the plane p, and normal vector $w/||w||_2$
- Projection of x onto the normal: $\frac{(x'-p)^T w}{\|w\|_2}$
- $(x'-p)^T w = x'^T w p^T w = x'^T w + b$ (since $p^T w + b = 0$)
- Signed distance between x' and Hyperplane H: $\frac{w^T x' + b}{\|w\|_2}$
- Taking into account of the label y: $d(x', H) = \frac{y(w^Tx' + b)}{\|w\|_{2}}$

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Maximize the Margin

We want to maximize the geometric margin:

maximize
$$\min_{i} d(x_i, H)$$
.

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

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

Let's remove the inner minimization problem by

maximize
$$M$$

subject to $\frac{y_i(w^Tx_i+b)}{\|w\|_2} \geqslant M$ for all i

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

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

It's equivalent to solving the minimization problem

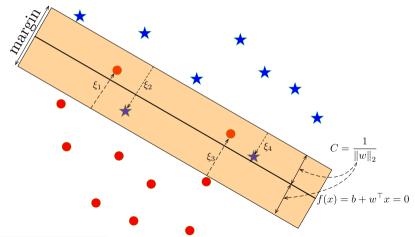
Note that $y_i(w^Tx_i + b)$ is the (functional) margin. The optimization finds the minimum norm solution which has a margin of at least 1 on all examples.

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Not linearly separable

What if the data is not linearly separable?

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



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Introduce slack variables ξ 's to penalize small margin:

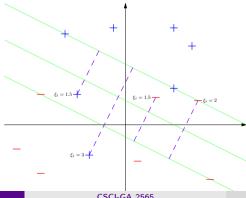
$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|w\|_2^2 + \frac{c}{n}\sum_{i=1}^n \xi_i \\ \text{subject to} & y_i(w^Tx_i + b) \geqslant 1 - \xi_i \quad \text{for all } i \\ & \xi_i \geqslant 0 \quad \text{for all } i \end{array}$$

- 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



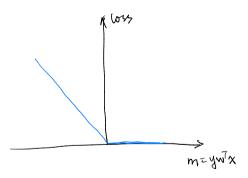
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Minimize the Hinge Loss

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Perceptron Loss

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

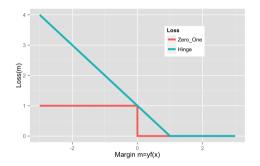


If we do ERM with this loss function, what happens?

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Hinge Loss

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



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

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SVM as an Optimization Problem

• The SVM optimization problem is equivalent to

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

which is equivalent to

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

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

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

Move the constraint into the objective:

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

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

Support Vector Machine

Using ERM:

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

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

Not differentiable because of the max

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

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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:

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

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

$$\nabla_{w}J(w) = \nabla_{w}\left(\frac{1}{n}\sum_{i=1}^{n}\ell(y_{i}w^{T}x_{i}) + \lambda||w||^{2}\right)$$
$$= \frac{1}{n}\sum_{i=1}^{n}\nabla_{w}\ell(y_{i}w^{T}x_{i}) + 2\lambda w$$

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"Gradient" of SVM Objective

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

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

By chain rule, we have

$$\nabla_{w}\ell(y_{i}w^{T}x_{i}) = \ell'(y_{i}w^{T}x_{i})y_{i}x_{i}$$

$$= \begin{cases} 0 & y_{i}w^{T}x_{i} > 1\\ -y_{i}x_{i} & y_{i}w^{T}x_{i} < 1\\ \text{undefined} & y_{i}w^{T}x_{i} = 1 \end{cases}$$

$$\nabla_{w} \ell \left(y_{i} w^{T} x_{i} \right) = \begin{cases} 0 & y_{i} w^{T} x_{i} > 1 \\ -y_{i} x_{i} & y_{i} w^{T} x_{i} < 1 \\ \text{undefined} & y_{i} w^{T} x_{i} = 1 \end{cases}$$

So

$$\nabla_{w}J(w) = \nabla_{w}\left(\frac{1}{n}\sum_{i=1}^{n}\ell\left(y_{i}w^{T}x_{i}\right) + \lambda||w||^{2}\right)$$

$$= \frac{1}{n}\sum_{i=1}^{n}\nabla_{w}\ell\left(y_{i}w^{T}x_{i}\right) + 2\lambda w$$

$$= \begin{cases} \frac{1}{n}\sum_{i:y_{i}w^{T}x_{i}<1}\left(-y_{i}x_{i}\right) + 2\lambda w & \text{all } y_{i}w^{T}x_{i} \neq 1\\ \text{undefined} & \text{otherwise} \end{cases}$$

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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?

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Subgradient

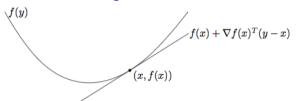
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First-Order Condition for Convex, Differentiable Function

• 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

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Subgradient Descent

• Move along the negative subgradient:

$$x^{t+1} = x^t - \eta g$$
 where $g \in \partial f(x^t)$ 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.

SVM objective function:

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

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 $j = 1, \dots, n$ (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.
- For convex optimization problem, we can also look into its dual problem.

The Lagrangian

The general [inequality-constrained] optimization problem is:

minimize
$$f_0(x)$$

subject to
$$f_i(x) \leq 0, i = 1, ..., m$$

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
- ullet Hard constraints o soft penalty (objective function)

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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)

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The Primal and the Dual

• For any primal form optimization problem,

minimize
$$f_0(x)$$

subject to $f_i(x) \leq 0$, $i = 1, ..., m$,

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

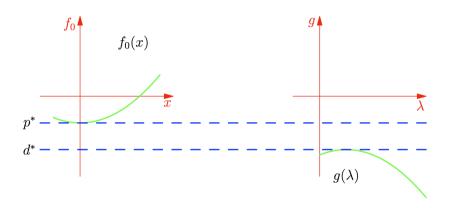
maximize
$$g(\lambda)$$

subject to $\lambda_i \ge 0$, $i = 1, ..., m$,

• The dual problem is always a convex optimization problem.

Weak Duality

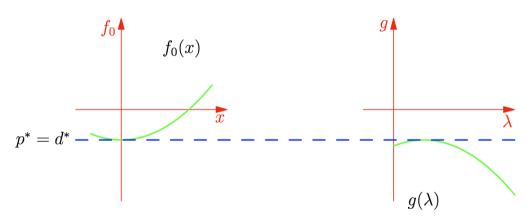
We always have **weak duality**: $p^* \geqslant d^*$.



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.

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

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

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

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

This condition is known as complementary slackness.

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The SVM Dual Problem

SVM Lagrange Multipliers

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

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

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

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

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Strong Duality by Slater's Constraint Qualification

The SVM optimization problem:

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

Slater's constraint qualification:

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

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SVM Dual Function: First Order Conditions

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

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

$$= \inf_{w, b, \xi} \left[\frac{1}{2} w^{T} w + \sum_{i=1}^{n} \xi_{i} \left(\frac{c}{n} - \alpha_{i} - \lambda_{i} \right) + \sum_{i=1}^{n} \alpha_{i} \left(1 - y_{i} \left[w^{T} x_{i} + b \right] \right) \right]$$

$$\partial_{w} L = 0 \iff w - \sum_{i=1}^{n} \alpha_{i} y_{i} x_{i} = 0 \iff w = \sum_{i=1}^{n} \alpha_{i} y_{i} x_{i}$$

$$\partial_{b} L = 0 \iff -\sum_{i=1}^{n} \alpha_{i} y_{i} = 0 \iff \sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

$$\partial_{\xi_{i}} L = 0 \iff \frac{c}{n} - \alpha_{i} - \lambda_{i} = 0 \iff \alpha_{i} + \lambda_{i} = \frac{c}{n}$$

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SVM Dual Function

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

$$\frac{1}{2}w^Tw = \frac{1}{2}\sum_{i,j=1}^n \alpha_i\alpha_jy_iy_jx_i^Tx_j$$

$$\sum_{i=1}^n \alpha_i(1-y_i[w^Tx_i+b]) = \sum_{i=1}^n \alpha_i - \sum_{i,j=1}^n \alpha_i\alpha_jy_iy_jx_j^Tx_i - b\sum_{i=1}^n \alpha_iy_i.$$

Putting it together, the dual function is

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

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The dual function is

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

• The dual problem is $\sup_{\alpha,\lambda \succ 0} g(\alpha,\lambda)$:

$$\sup_{\alpha,\lambda} \qquad \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{j}^{T} x_{i}$$
s.t.
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

$$\alpha_{i} + \lambda_{i} = \frac{c}{n} \quad \alpha_{i}, \lambda_{i} \geqslant 0, \ i = 1, \dots, n$$

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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: $f_i(x) \leq 0 \quad \forall i$
- 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:

$$\sup_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{j}^{T} x_{i}$$
s.t.
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

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

- 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?

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Complementary Slackness Conditions

• Recall our primal constraints and Lagrange multipliers:

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

- 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.

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

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 $y_i f^*(x) \ge 1$.
- If $\alpha_i^* \in (0, \frac{c}{n})$, then $\xi_i^* = 0$, which implies $1 y_i f^*(x_i) = 0$.

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Complementary Slackness Results: Summary

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

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

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

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

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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**.
- ullet Few margin errors or "on the margin" examples \Longrightarrow sparsity in input examples.

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Kernelization

Dual Problem: Dependence on x through inner products

SVM Dual Problem:

$$\sup_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{j}^{T} x_{i}$$
s.t.
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

$$\alpha_{i} \in \left[0, \frac{c}{n}\right] \ i = 1, \dots, n.$$

- 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 $x_i^T x_i$ by other products...
- This is a "kernelized" objective function.

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Feature Maps

The Input Space ${\mathfrak X}$

- ullet Our general learning theory setup: no assumptions about ${\mathcal X}$
- But $\mathfrak{X} = \mathbb{R}^d$ 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 :

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

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

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The Input Space $\mathfrak X$

- 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 *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 X to a vector in R^d is called **feature extraction** or **featurization**.

Raw Input

Feature Vector

$$\mathcal{X} \xrightarrow{x}$$
 Feature $\phi(x)$ \mathbb{R}^{a}

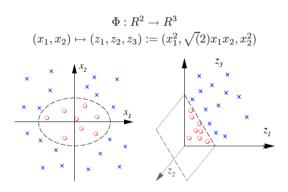
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Linear Models with Explicit Feature Map

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

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

Geometric Example: Two class problem, nonlinear boundary



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

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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...

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

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Non-monotonicity: The Issue

- Feature Map: $\phi(x) = [1, temperature(x)]$
- 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.

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

Non-monotonicity: Solution 1

• Transform the input:

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

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.

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

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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

• Smooth nonlinear transformation:

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

- ullet log (\cdot) good for values with large dynamic ranges
- Discretization (a discontinuous transformation):

$$\phi(x) = (1[0 \le N(x) < 10], 1[10 \le N(x) < 100], \ldots)$$

Small buckets allow quite flexible relationship

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

Interactions: The Issue

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

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

- 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.

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Interactions: Approach 1

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

$$weight(kg) = 52 + 1.9 [height(in) - 60]$$

• 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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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.

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

- Suppose we start with $x = (1, x_1, \dots, x_d) \in \mathbb{R}^{d+1} = \mathfrak{X}$.
- 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_1x_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.

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The Kernel Trick

SVM with Explicit Feature Map

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

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

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

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SVM Dual Problem

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

$$\begin{aligned} & \underset{i=1}{\text{maximize}} & & \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} \psi \left(x_{j} \right)^{T} \psi \left(x_{i} \right) \\ & \text{s.t.} & & \sum_{i=1}^{n} \alpha_{i} y_{i} = 0 \quad \text{and} \quad \alpha_{i} \in \left[0, \frac{c}{n} \right] \quad \forall i. \end{aligned}$$

• If α^* is an optimal value, then

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

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

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Compute the Inner Products

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

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

The inner product is

$$\psi(x)^{T}\psi(x') = x_{1}^{2}x_{1}'^{2} + (\sqrt{2}x_{1}x_{2})(\sqrt{2}x_{1}'x_{2}') + x_{2}^{2}x_{2}'^{2}$$

$$= (x_{1}x_{1}')^{2} + 2(x_{1}x_{1}')(x_{2}x_{2}') + (x_{2}x_{2}')^{2}$$

$$= (x_{1}x_{1}' + x_{2}x_{2}')^{2}$$

$$= (x^{T}x')^{2}$$

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

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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

$$\psi(x)^T \psi(x') = (1 + x^T x')^2$$
 (check).

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

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

(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)

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Kernel Function

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The Kernel Function

- $\bullet \ \, \textbf{Input space} \colon \, \mathfrak{X}$
- Feature space: \mathcal{H} (a Hilbert space, e.g. \mathbb{R}^d)
- Feature map: $\psi: \mathfrak{X} \to \mathcal{H}$
- 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:

maximize
$$\sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} \psi(x_{j})^{T} \psi(x_{i})$$

s.t.
$$\sum_{i=1}^{n} \alpha_i y_i = 0$$
 and $\alpha_i \in \left[0, \frac{c}{n}\right] \quad \forall i$.

Prediction:

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

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Definition

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

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

• 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} :

$$\begin{aligned} \text{maximize}_{\alpha} & & \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathcal{K}_{ij} \\ \text{s.t.} & & \sum_{i=1}^{n} \alpha_{i} y_{i} = 0 \quad \text{and} \quad \alpha_{i} \in \left[0, \frac{c}{n}\right] \ i = 1, \dots, n. \end{aligned}$$

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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.

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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?

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How to Get Kernels?

- Explicitly construct $\psi(x): \mathcal{X} \to \mathbb{R}^d$ (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.

Definition

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

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

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: $\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j k(x_i, x_j) \ge 0$ given $\alpha_i \in \mathbb{R} \ \forall i$.

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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 , $k_2 : \mathcal{X} \times \mathcal{X} \to \mathsf{R}$ are pd kernels. Then so are the following:

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

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

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Linear Kernel

- Input space: $\mathfrak{X} = \mathbb{R}^d$
- Feature space: $\mathcal{H} = \mathbb{R}^d$, with standard inner product
- Feature map

$$\psi(x) = x$$

• Kernel:

$$k(x,x') = x^T x'$$

Quadratic Kernel in R^d

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

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

• Then for $\forall x, x' \in \mathbb{R}^d$

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

= $\langle x, x' \rangle + \langle x, x' \rangle^2$

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

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Polynomial Kernel in R^d

- Input space $\mathfrak{X} = \mathbb{R}^d$
- Kernel function:

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

- \bullet 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 $\mathfrak{X} = \mathbb{R}^d$

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

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

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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:

$$\sup_{\alpha \in \mathbb{R}^n} \qquad \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_j^T x_i$$
s.t.
$$\sum_{i=1}^n \alpha_i y_i = 0$$

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

- 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, $w^* \in \text{span}(x_1, \dots, x_n)$.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Note that for any $w \in \text{span}(x_1, \dots, x_n)$, 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:

- 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?

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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 $(d \gg n)$.

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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.

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The Representer Theorem (Optional)

• Generalized objective:

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

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

$$w^* = \underset{w \in \operatorname{span}(x_1, \dots, x_n)}{\operatorname{arg\,min}} R(\|w\|) + L(\langle w, x_1 \rangle, \dots, \langle w, x_n \rangle).$$

• So we can reparameterize as before:

$$\alpha^* = \operatorname*{arg\,min}_{\alpha \in \mathbb{R}^n} R\left(\left\| \sum_{i=1}^n \alpha_i x_i \right\| \right) + L\left(\left\langle \sum_{i=1}^n \alpha_i x_i, x_1 \right\rangle, \dots, \left\langle \sum_{i=1}^n \alpha_i x_i, x_n \right\rangle \right).$$

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

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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.
- ullet Once kernelized, we can apply the kernel trick: doesn't need to represent $\varphi(x)$ explicitly.

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