Recap for Midterm

Spring 2020

Contents

- Learning Theory Framework
- 2 Regularization
- Optimization
- 4 Classification
- 5 The Representer Theorem and Kernelization

Learning Theory Framework

Some Formalization

The Spaces

• \mathfrak{X} : input space

• y: outcome space

A: action space

Prediction Function (or "decision function")

A prediction function (or decision function) gets input $x \in \mathcal{X}$ and produces an action $a \in \mathcal{A}$:

$$f: \mathcal{X} \rightarrow \mathcal{A}$$
 $x \mapsto f(x)$

Loss Function

A loss function evaluates an action in the context of the outcome y.

$$\ell: \mathcal{A} \times \mathcal{Y} \rightarrow \mathbf{R}$$
 $(a,y) \mapsto \ell(a,y)$

Risk and the Bayes Prediction Function

Definition

The **risk** of a prediction function $f: \mathcal{X} \to \mathcal{A}$ is

$$R(f) = \mathbb{E}\ell(f(x), y).$$

In words, it's the **expected loss** of f on a new example (x,y) drawn randomly from $P_{\mathfrak{X}\times \mathfrak{Y}}$.

Definition

A Bayes prediction function $f^*: \mathcal{X} \to \mathcal{A}$ is a function that achieves the *minimal risk* among all possible functions:

$$f^* \in \operatorname*{arg\,min}_f R(f)$$
,

where the minimum is taken over all functions from \mathfrak{X} to \mathcal{A} .

• The risk of a Bayes prediction function is called the Bayes risk.

Bayes Prediction Function

- If loss function is L2, then $f^*(x) = E[Y|X = x]$
- if loss function is L1, then $f^*(x)$ is the median of the distribution of Y conditioned on X = x.
- If $\mathcal Y$ is discrete and loss function is 0-1 loss, then $f^*(x) = \underset{c \in \mathcal Y}{\operatorname{argmax}} \ p(y=c|x)$

Question: Let x be sampled uniformly from $\{-100, -99, \dots, 99, 100\}$. For every sample x_i , y_i is generated as $y_i = x_i + \eta$, $\eta \sim \mathcal{N}(0, \sigma)$, $\sigma > 0$. What is the Bayes prediction function under L_2 and L_1 loss?

The Empirical Risk

- Let $\mathcal{D}_n = ((x_1, y_1), \dots, (x_n, y_n))$ be drawn i.i.d. from $\mathcal{P}_{\mathcal{X} \times \mathcal{Y}}$.
- The **empirical risk** of $f: \mathcal{X} \to \mathcal{A}$ with respect to \mathcal{D}_n is

$$\hat{R}_n(f) = \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i).$$

• A function \hat{f} is an empirical risk minimizer if

$$\hat{f} \in \operatorname*{arg\,min}_{f} \hat{R}_{n}(f),$$

where the minimum is taken over all functions.

But unconstrained ERM can overfit.

Constrained Empirical Risk Minimization

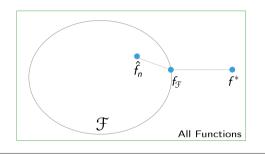
- Hypothesis space \mathcal{F} , a set of [prediction] functions mapping $\mathcal{X} \to \mathcal{A}$
- ullet Empirical risk minimizer (ERM) in ${\mathfrak F}$ is

$$\hat{f}_n \in \underset{f \in \mathcal{F}}{\operatorname{arg\,min}} \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i).$$

ullet Risk minimizer in $\mathcal F$ is $f_{\mathcal F}^*\in \mathcal F$, where

$$f_{\mathcal{F}}^* \in \underset{f \in \mathcal{F}}{\operatorname{arg\,min}} \mathbb{E}\ell(f(x), y).$$

Error Decomposition



$$f^* = \underset{f}{\operatorname{arg \, min}} \mathbb{E}\ell(f(X), Y)$$

$$f_{\mathcal{F}} = \underset{f \in \mathcal{F}}{\operatorname{arg \, min}} \mathbb{E}\ell(f(X), Y))$$

$$\hat{f}_n = \underset{f \in \mathcal{F}}{\operatorname{arg \, min}} \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i)$$

- Approximation Error (of \mathfrak{F}) = $R(f_{\mathfrak{F}}) R(f^*)$
- Estimation error (of \hat{f}_n in \mathcal{F}) = $R(\hat{f}_n) R(f_{\mathcal{F}})$

Excess Risk Decomposition for ERM

• The excess risk of the ERM \hat{f}_n can be decomposed:

Excess
$$\operatorname{Risk}(\hat{f}_n) = R(\hat{f}_n) - R(f^*)$$

$$= \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}.$$

Optimization Error

- In practice, we don't find the ERM $\hat{f}_n \in \mathcal{F}$.
- ullet Optimization algorithm returns $\widetilde{f}_n \in \mathcal{F}$, which we hope is good enough.
- Optimization error: If \tilde{f}_n is the function our optimization method returns, and \hat{f}_n is the empirical risk minimizer, then

Optimization Error =
$$R(\tilde{f}_n) - R(\hat{f}_n)$$
.

Extended decomposition:

Excess Risk
$$(\tilde{f}_n) = R(\tilde{f}_n) - R(f^*)$$

$$= \underbrace{R(\tilde{f}_n) - R(\hat{f}_n)}_{\text{optimization error}} + \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}$$

Question

Select true of false for each of the following statements:

- Approximation Error is a Random Variable
- Estimation Error is a Random Variable
- Optimization Error is a Random Variable.
- If the hypothesis space consists of all possible functions functions, then approximation error is non-zero.
- 5 Estimation Error can be negative.
- Optimization Error can be negative.
- The empirical risk of the ERM, $\hat{R}(\hat{f})$, is an unbiased estimator of the risk of the ERM $R(\hat{f})$. Does your answer change if it's a $\hat{R}(f)$ where f is independent of training data?

Question

For each, use \leq , \geqslant , or = to determine the relationship between the two quantities, or if the relationship cannot be determined. Throughout assume $\mathcal{F}_1, \mathcal{F}_2$ are hypothesis spaces with $\mathcal{F}_1 \subset \mathcal{F}_2$, and assume we are working with a fixed loss function ℓ .

- The estimation errors of two decision functions f_1 , f_2 that minimize the empirical risk over the same hypothesis space, where f_2 uses 5 extra data points.
- ② The approximation errors of the two decision functions f_1 , f_2 that minimize risk with respect to \mathcal{F}_1 , \mathcal{F}_2 , respectively (i.e., $f_1 = f_{\mathcal{F}_1}$ and $f_2 = f_{\mathcal{F}_2}$).
- **3** The empirical risks of two decision functions f_1 , f_2 that minimize the empirical risk over \mathcal{F}_1 , \mathcal{F}_2 , respectively. Both use the same fixed training data.
- The estimation errors (for \mathcal{F}_1 , \mathcal{F}_2 , respectively) of two decision functions f_1 , f_2 that minimize the empirical risk over \mathcal{F}_1 , \mathcal{F}_2 , respectively.
- **5** The risk of two decision functions f_1 , f_2 that minimize the empirical risk over \mathcal{F}_1 , \mathcal{F}_2 , respectively.

Solution

- **1** Roughly speaking, more data is better, so we would tend to expect that f_2 will have lower estimation error. That said, this is not always the case, so the relationship cannot be determined.
- ② The approximation error of f_1 will be larger.
- **1** The empirical risk of f_1 will be larger.
- Roughly speaking, increasing the hypothesis space should increase the estimation error since the approximation error will decrease, and we expect to need more data. That said, this is not always the case, so the answer is the relationship cannot be determined.
- Cannot be determined.

Regularization

Constrained Empirical Risk Minimization

Constrained ERM (Ivanov regularization)

For complexity measure $\Omega: \mathcal{F} \to [0, \infty)$ and fixed $r \geqslant 0$,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$
s.t. $\Omega(f) \leqslant r$

- Choose r using validation data or cross-validation.
- Each r corresponds to a different hypothesis spaces. Could also write:

$$\min_{f \in \mathcal{F}_r} \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i)$$

Penalized Empirical Risk Minimization

Penalized ERM (Tikhonov regularization)

For complexity measure $\Omega: \mathcal{F} \to [0, \infty)$ and fixed $\lambda \geqslant 0$,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \lambda \Omega(f)$$

- Choose λ using validation data or cross-validation.
- (Ridge regression in homework is of this form.)

Ridge Regression: Workhorse of Modern Data Science

Ridge Regression (Tikhonov Form)

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

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

where $||w||_2^2 = w_1^2 + \cdots + w_d^2$ is the square of the ℓ_2 -norm.

Ridge Regression (Ivanov Form)

The ridge regression solution for complexity parameter $r \ge 0$ is

$$\hat{w} = \arg\min_{\|w\|_{2}^{2} \leq r^{2}} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^{T} x_{i} - y_{i} \right\}^{2}.$$

Lasso Regression: Workhorse (2) of Modern Data Science

Lasso Regression (Tikhonov Form)

The lasso regression solution for regularization parameter $\lambda \geqslant 0$ is

$$\hat{w} = \underset{w \in \mathbb{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^n \left\{ w^T x_i - y_i \right\}^2 + \lambda ||w||_1,$$

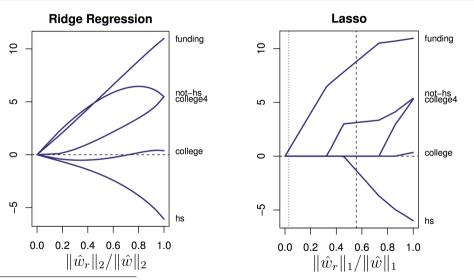
where $||w||_1 = |w_1| + \cdots + |w_d|$ is the ℓ_1 -norm.

Lasso Regression (Ivanov Form)

The lasso regression solution for complexity parameter $r \ge 0$ is

$$\hat{w} = \underset{\|w\|_{1} \leq r}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \{w^{T} x_{i} - y_{i}\}^{2}.$$

Ridge vs. Lasso: Regularization Paths



Modified from Hastie, Tibshirani, and Wainwright's Statistical Learning with Sparsity, Fig 2.1. About predicting crime in 50 US cities.

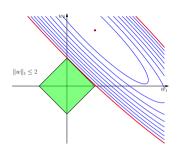
DS-GA 1003 / CSCI-GA 2567 Spring 2020

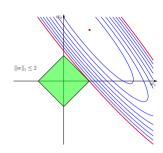
20 / 50

Linearly Dependent Features: Take Away

- For identical features
 - ℓ_1 regularization spreads weight arbitrarily (all weights same sign)
 - ullet ℓ_2 regularization spreads weight evenly
- Linearly related features
 - \bullet ℓ_1 regularization chooses variable with larger scale, 0 weight to others
 - ullet ℓ_2 prefers variables with larger scale spreads weight proportional to scale

Correlated Features, ℓ_1 Regularization





- Intersection could be anywhere on the top right edge.
- Minor perturbations (in data) can drastically change intersection point very unstable solution.
- Makes division of weight among highly correlated features (of same scale) seem arbitrary.
 - If $x_1 \approx 2x_2$, ellipse changes orientation and we hit a corner. (Which one?)

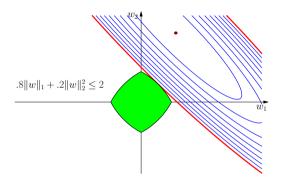
Elastic Net

• The elastic net combines lasso and ridge penalties:

$$\hat{w} = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \left\{ w^T x_i - y_i \right\}^2 + \lambda_1 \|w\|_1 + \lambda_2 \|w\|_2^2$$

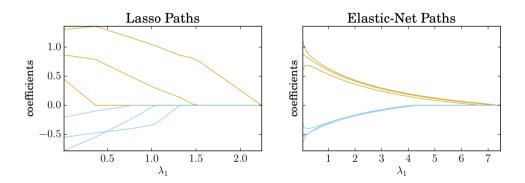
• We expect correlated random variables to have similar coefficients.

Highly Correlated Features, Elastic Net Constraint



• Elastic net solution is closer to $w_2 = w_1$ line, despite high correlation.

Elastic Net Results on Model



- Lasso on left; Elastic net on right.
- Ratio of ℓ_2 to ℓ_1 regularization roughly 2:1.

Elastic Net Summary

- With uncorrelated features, we can get sparsity.
- Among correlated features (same scale), we spread weight more evenly.

Question on correlated features

We solve lasso and ridge regression where input lives in \mathbb{R}^4 . The first two features of all the input vector are duplicates of each other, or $x_{i1} = x_{i2}$ for all i. Consider the following weight vectors:

- $(0, 1.2, 6.7, 2.1)^T$
- $(0.6, 0.6, 6.7, 2.1)^T$
- $(1.2, 0, 6.7, 2.1)^T$
- $(-0.1, 1.3, 6.7, 2.1)^T$

Which of them are valid solution for a) Ridge Regression and b) Lasso Regression?

Finding Lasso Solution

- Many options.
- Convert to quadratic program using positive/negative parts

$$\min_{w^+,w^-} \quad \sum_{i=1}^n \left(\left(w^+ - w^- \right)^T x_i - y_i \right)^2 + \lambda 1^T \left(w^+ + w^- \right)$$
subject to $w_i^+ \geqslant 0$ for all i $w_i^- \geqslant 0$ for all i ,

- Coordinate descent
 - Lasso has closed form solution for coordinate minimizers!
- Subgradient descent

Optimization

Gradient Descent for Empirical Risk and Averages

- Suppose we have a hypothesis space of functions $\mathcal{F} = \{f_w : \mathcal{X} \to \mathcal{A} \mid w \in \mathbf{R}^d\}$
 - Parameterized by $w \in \mathbb{R}^d$.
- ERM is to find w minimizing

$$\hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^n \ell(f_w(x_i), y_i)$$

- Suppose $\ell(f_w(x_i), y_i)$ is differentiable as a function of w.
- Then we can do gradient descent on $\hat{R}_n(w)$...

Gradient Descent: How does it scale with n?

• At every iteration, we compute the gradient at current w:

$$\nabla \hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^n \nabla_w \ell(f_w(x_i), y_i)$$

- We have to touch all n training points to take a single step. [O(n)]
- What if we just use an estimate of the gradient?

Minibatch Gradient

• The full gradient is

$$\nabla \hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^n \nabla_w \ell(f_w(x_i), y_i)$$

- It's an average over the **full batch** of data $\mathcal{D}_n = \{(x_1, y_1), \dots, (x_n, y_n)\}.$
- Let's take a random subsample of size *N* (called a **minibatch**):

$$(x_{m_1}, y_{m_1}), \ldots, (x_{m_N}, y_{m_N})$$

• The minibatch gradient is

$$\nabla \hat{R}_{N}(w) = \frac{1}{N} \sum_{i=1}^{N} \nabla_{w} \ell(f_{w}(x_{m_{i}}), y_{m_{i}})$$

• Minibatch gradient is an unbiased estimate of full-batch gradient: $\mathbb{E}\left[\nabla\hat{R}_{N}(w)\right] = \nabla\hat{R}_{n}(w)$

How big should minibatch be?

- Tradeoffs of minibatch size:
 - Bigger $N \implies$ Better estimate of gradient, but slower (more data to touch)
 - Smaller $N \implies$ Worse estimate of gradient, but can be quite fast
- Even N = 1 works, it's traditionally called **stochastic gradient descent** (SGD).
- Quality of minibatch estimate depends on
 - size of minibatch
 - but is independent of full dataset size n

Classification

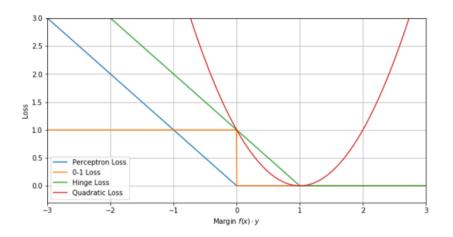
The Margin

Definition

The margin (or functional margin) for predicted score \hat{y} and true class $y \in \{-1, 1\}$ is $y\hat{y}$.

- The margin often looks like yf(x), where $f: \mathcal{X} \to \mathbf{R}$ is our hypothesis.
- The margin is a measure of how correct we are.
 - If y and \hat{y} are the same sign, prediction is **correct** and margin is **positive**.
 - If y and \hat{y} have different sign, prediction is **incorrect** and margin is **negative**.
- We want to maximize the margin.

Classification Losses



Support Vector Machine

- 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)
- Loss $\ell(m) = \max\{1 m, 0\}$
- The SVM prediction function is the solution to

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

SVM as a Quadratic Program

The SVM optimization problem is equivalent to

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

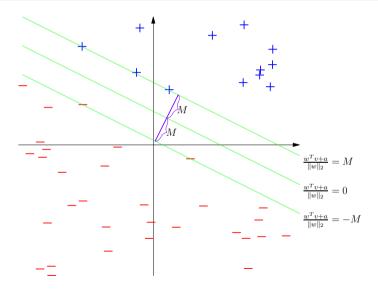
- Differentiable objective function
- n+d+1 unknowns and 2n affine constraints.
- A quadratic program that can be solved by any off-the-shelf QP solver.
- We arrived at this optimization problem also from a geometric prospective.

Linear Separability and Hard Margin SVM

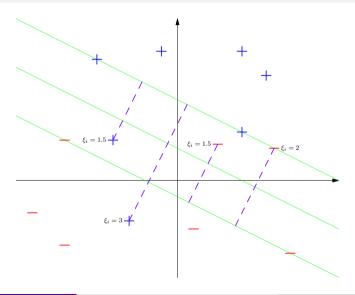
Definition (Linear Separability)

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.

Maximum Margin Separating Hyperplane



Soft Margin SVM (unlabeled points have $\xi_i = 0$)



The Representer Theorem and Kernelization

General Objective Function for Linear Hypothesis Space (Details)

Generalized objective:

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

where

- $w, x_1, ..., x_n \in \mathcal{H}$ for some Hilbert space \mathcal{H} . (We typically have $\mathcal{H} = \mathbf{R}^d$.)
- $\|\cdot\|$ is the norm corresponding to the inner product of \mathcal{H} . (i.e. $\|w\| = \sqrt{\langle w, w \rangle}$)
- $R:[0,\infty)\to \mathbf{R}$ is nondecreasing (**Regularization term**), and
- $L: \mathbb{R}^n \to \mathbb{R}$ is arbitrary (Loss term).
- Ridge regression and SVM are of this form.
- What if we use lasso regression? No! ℓ_1 norm does not correspond to an inner product.

The Representer Theorem

Let $J(w) = R(||w||) + L(\langle w, x_1 \rangle, \dots, \langle w, x_n \rangle)$ under conditions described above.

Theorem (Representer Theorem)

If J(w) has a minimizer, then it has a minimizer of the form

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

If R is strictly increasing, then all minimizers have this form.

Basic idea of proof:

- Let $M = \operatorname{span}(x_1, \dots, x_n)$. [the "span of the data"]
- Let $w = \text{Proj}_M w^*$, for some minimizer w^* of J(w).
- Then $\langle w, x_i \rangle = \langle w^*, x_i \rangle$, so loss part doesn't change.
- $||w|| \le ||w^*||$, since projection reduces norm. So regularization piece never increases.

Reparametrization with Representer Theorem

- Original plan:
 - Find $w^* \in \operatorname{arg\,min}_{w \in \mathcal{H}} R(\|w\|) + L(\langle w, x_1 \rangle, \dots, \langle w, x_n \rangle)$
 - Predict with $\hat{f}(x) = \langle w^*, x \rangle$.
- Plugging in result of representer theorem, it's equivalent to
 - Find $\alpha^* \in \operatorname{arg\,min}_{\alpha \in \mathbb{R}^n} R\left(\sqrt{\alpha^T K \alpha}\right) + L(K \alpha)$
 - Predict with $\hat{f}(x) = k_x^T \alpha^*$, where

$$K = \begin{pmatrix} \langle x_1, x_1 \rangle & \cdots & \langle x_1, x_n \rangle \\ \vdots & \ddots & \ddots \\ \langle x_n, x_1 \rangle & \cdots & \langle x_n, x_n \rangle \end{pmatrix} \quad \text{and} \quad k_x = \begin{pmatrix} \langle x_1, x \rangle \\ \vdots \\ \langle x_n, x \rangle \end{pmatrix}$$

• Every element $x \in \mathcal{H}$ occurs inside an inner products with a training input $x_i \in \mathcal{H}$.

Kernelization

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.

• Here we are using $\psi(x) = x$. Thus finding

$$\alpha^* \in \operatorname*{arg\,min}_{\alpha \in \mathbf{R}^n} R\left(\sqrt{\alpha^T K \alpha}\right) + L(K \alpha)$$

and making predictions with $\hat{f}(x) = k_x^T \alpha^*$ is a **kernelization** of finding

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

and making predictions with $\hat{f}(x) = \langle w^*, x \rangle$.

Kernelization

- Once we have kernelized:
 - $\alpha^* \in \operatorname{arg\,min}_{\alpha \in \mathbf{R}^n} R\left(\sqrt{\alpha^T K \alpha}\right) + L(K \alpha)$
 - $\hat{f}(x) = k_x^T \alpha^*$
- We can do the "kernel trick".
- Replace each $\langle x, x' \rangle$ by k(x, x'), for any kernel function k, where $k(x, x') = \langle \psi(x), \psi(x') \rangle$.
- Predictions

$$\hat{f}(x) = \sum_{i=1}^{n} \alpha_i^* k(x_i, x)$$

The Kernel Function: Why do we need this?

- Feature map: $\psi: \mathcal{X} \to \mathcal{H}$
- The kernel function corresponding to ψ is

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

- Why introduce this new notation k(x, x')?
- We can often evaluate k(x,x') without explicitly computing $\psi(x)$ and $\psi(x')$.
- For large feature spaces, can be much faster.

Kernelized SVM (From Lagrangian Duality)

• Kernelized SVM from computing the Lagrangian Dual Problem:

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

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

• If α^* is an optimal value, then

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

• Note that the prediction function is also kernelized.

Sparsity in the Data from Complementary Slackness

Kernelized predictions given by

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

• By a Lagrangian duality analysis (specifically from complementary slackness), we find

$$y_i \hat{f}(x_i) < 1 \implies \alpha_i^* = \frac{c}{n}$$

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

- So we can leave out any x_i "on the good side of the margin" $(y_i\hat{f}(x_i) > 1)$.
- x_i 's that we must keep, because $\alpha_i^* \neq 0$, are called support vectors.