The Representer Theorem and Kernelization

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Contents

Solutions in the "span of the data," and so what?

SVM solution is in the "span of the data"

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

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

- Given solution α^* to dual, primal solution is $w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i$.
- 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 #4):

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

where X is the design matrix, with $x_1, \ldots, x_n$ 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 #4):

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

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

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

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

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

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

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

- How can we conveniently write an optimization problem over the span of some vectors?

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

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

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

- 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 ($d \gg n$).

What's next?

- For SVM and ridge regression, we found that the solution is in the span of the data.
  - derived in two rather ad-hoc ways
- Up next: The Representer Theorem, which shows that this "span of the data" result occurs far more generally, and we prove it using basic linear algebra.

Math Review: Inner Product Spaces and Projections (Hilbert Spaces)

Inner Product Space (or "Pre-Hilbert" Spaces)

An **inner product space** (over reals) is a vector space $\mathcal{V}$ and an **inner product**, which is a mapping

$$\langle \cdot, \cdot \rangle : \mathcal{V} \times \mathcal{V} \to \mathbf{R}$$

that has the following properties $\forall x, y, z \in \mathcal{V}$ and $a, b \in \mathbf{R}$:

- Symmetry: $\langle x, y \rangle = \langle y, x \rangle$
- Linearity: $\langle ax + by, z \rangle = a \langle x, z \rangle + b \langle y, z \rangle$
- Positive-definiteness: $\langle x, x \rangle \geqslant 0$ and $\langle x, x \rangle = 0 \iff x = 0$.

Norm from Inner Product

For an inner product space, we define a norm as

$$\|x\| = \sqrt{\langle x, x \rangle}.$$

Example

$\mathbf{R}^d$ with standard Euclidean inner product is an inner product space:

$$\langle x, y \rangle := x^T y \qquad \forall x, y \in \mathbf{R}^d.$$

Norm is

$$\|x\| = \sqrt{x^T x}.$$

What norms can we get from an inner product?

Theorem (Parallelogram Law)

A norm $\|\cdot\|$ can be written in terms of an inner product on $\mathcal{V}$ iff $\forall x, x' \in \mathcal{V}$

$$2\|x\|^2 + 2\|x'\|^2 = \|x + x'\|^2 + \|x - x'\|^2,$$

*and if it can, the inner product is given by the **polarization identity***

$$\langle x, x' \rangle = \frac{\|x\|^2 + \|x'\|^2 - \|x - x'\|^2}{2}.$$

Example

ℓ_1 norm on $\mathbf{R}^d$ is NOT generated by an inner product. [Exercise]

Is ℓ_2 norm on $\mathbf{R}^d$ generated by an inner product?

Orthogonality (Definitions)

Definition

Two vectors are **orthogonal** if $\langle x, x' \rangle = 0$. We denote this by $x \perp x'$.

Definition

x is orthogonal to a set S, i.e. $x \perp S$, if $x \perp s$ for all $x \in S$.

Pythagorean Theorem

Theorem (Pythagorean Theorem)

If $x \perp x'$, *then* $\|x+x'\|^2 = \|x\|^2 + \|x'\|^2$.

Proof.

We have

$$
\begin{aligned}
\|x+x'\|^2 &= \langle x+x', x+x' \rangle \\
&= \langle x,x \rangle + \langle x,x' \rangle + \langle x',x \rangle + \langle x',x' \rangle \\
&= \|x\|^2 + \|x'\|^2.
\end{aligned}
$$

□

Projection onto a Plane (Rough Definition)

- Choose some $x \in \mathcal{V}$.
- Let M be a subspace of inner product space $\mathcal{V}$.
- Then m_0 is the **projection of** x **onto** M**,**
  - if $m_0 \in M$ and is the closest point to x in M.
- In math: For all $m \in M$,

$$\|x - m_0\| \leqslant \|x - m\|.$$

Hilbert Space

- Projections exist for all finite-dimensional inner product spaces.
- We want to allow infinite-dimensional spaces.
- Need an extra condition called **completeness**.
- A space is **complete** if all Cauchy sequences in the space converge.

Definition

A **Hilbert space** is a complete inner product space.

Example

Any finite dimensional inner product space is a Hilbert space.

Theorem (Classical Projection Theorem)

- *$\mathcal{H}$ a Hilbert space*
- *M a closed subspace of $\mathcal{H}$ (picture a hyperplane through the origin)*
- *For any $x \in \mathcal{H}$, there **exists a unique** $m_0 \in M$ for which*

$$\|x - m_0\| \leqslant \|x - m\| \; \forall m \in M.$$

- *This m_0 is called the **[orthogonal] projection of** x **onto** M.*
- *Furthermore, $m_0 \in M$ is the projection of x onto M iff*

$$x - m_0 \perp M.$$

Projection Reduces Norm

Theorem

Let M be a closed subspace of $\mathcal{H}$. For any $x \in \mathcal{H}$, let $m_0 = Proj_M x$ be the projection of x onto M. Then

$$\|m_0\| \leqslant \|x\|,$$

with equality only when $m_0 = x$.

Proof.

$$\begin{aligned}
\|x\|^2 &= \|m_0 + (x - m_0)\|^2 \text{ (note: } x - m_0 \perp m_0 \text{ by Projection theorem)} \\
&= \|m_0\|^2 + \|x - m_0\|^2 \text{ by Pythagorean theorem} \\
\|m_0\|^2 &= \|x\|^2 - \|x - m_0\|^2
\end{aligned}$$

Then $\|x - m_0\|^2 \geqslant 0$ implies $\|m_0\|^2 \leqslant \|x\|^2$. If $\|x - m_0\|^2 = 0$, then $x = m_0$, by definition of norm. $\square$

The Representer Theorem

Generalize from SVM Objective

- SVM objective:

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

- **Generalized objective**:

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

  where

  - $R : [0, \infty) \to \mathbf{R}$ is nondecreasing (**Regularization term**)
  - and $L : \mathbf{R}^n \to \mathbf{R}$ is arbitrary. (**Loss term**)

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

  - $w, x_1, \dots, x_n \in \mathcal{H}$ 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
  - $L : \mathbf{R}^n \to \mathbf{R}$ is arbitrary (**Loss term**).

General Objective Function for Linear Hypothesis Space (Details)

- **Generalized objective**:

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

- What's "linear"?
- The prediction/score function $x \mapsto \langle w, x \rangle$ is linear – in what?
  - in parameter vector w, and
  - in the feature vector x.
- Why? [Real-valued] inner products are linear in each argument.
- **The important part is the linearity in the parameter** w.

General Objective Function for Linear Hypothesis Space (Details)

- **Generalized objective**:

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

- Ridge regression and SVM are of this form. (Verify this!)
- What if we penalize with $\lambda\|w\|_2$ instead of $\lambda\|w\|_2^2$? Yes!.
- What if we use lasso regression? No! ℓ_1 norm does not correspond to an inner product.

The Representer Theorem: Quick Summary

- **Generalized objective**:

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

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

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

- So we can reparameterize as before:

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

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

The Representer Theorem

Theorem (Representer Theorem)

Let

$$J(w) = R(\|w\|) + L(\langle w, x_1 \rangle, \ldots, \langle w, x_n \rangle),$$

where

- $w, x_1, \ldots, x_n \in \mathcal{H}$ *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*
- $L : \mathbf{R}^n \to \mathbf{R}$ *is arbitrary **(Loss term)**.*

Then

- *If* $M = \text{span}(x_1, \ldots, x_n)$*, then* $J(\text{Proj}_M w) \leqslant J(w)$ *for any* $w \in \mathcal{H}$.
- *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. (Proof in homework.)*

The Representer Theorem (Proof)

1. Fix any $w \in \mathcal{H}$.
2. Let $w_M = \text{Proj}_M w$.
3. Residual $w - w_M$ is orthogonal to x for all $x \in M$.
4. $\langle w, x_i \rangle = \langle w_M + w - w_M, x_i \rangle = \langle w_M, x_i \rangle + \langle w - w_M, x_i \rangle = \langle w_M, x_i \rangle \ \forall i$.
5. $L(\langle w, x_1 \rangle, \ldots, \langle w, x_n \rangle) = L(\langle w_M, x_1 \rangle, \ldots, \langle w_M, x_n \rangle)$.
6. Projections decrease norms $\implies \|w_M\| \leqslant \|w\|$.
7. Since R is nondecreasing, $R(\|w_M\|) \leqslant R(\|w\|)$.
8. $J(w_M) \leqslant J(w)$. [Proves first result.]
9. If w^* minimizes $J(w)$, then $w_M^* = \text{Proj}_M w^*$ is also a minimizer, since $J(w_M^*) \leqslant J(w^*)$.
10. So $\exists \alpha$ s.t. $w_M^* = \sum_{i=1}^n \alpha_i x_i$ is a minimizer of $J(w)$.

Q.E.D.

Sufficient Condition for Existence of a Minimizer

Theorem

[a] *Let*

$$J(w) = R(\|w\|) + L(\langle w, x_1 \rangle, \ldots, \langle w, x_n \rangle),$$

and let $M = \text{span}(x_1, \ldots, x_n)$. *Then under the same conditions given in the Representer theorem, if* w_M^* *minimizes* $J(w)$ ***over the set*** M, *then* w_M^* *minimizes* $J(w)$ *over all* $\mathcal{H}$.

[a] Thanks to Mingsi Long for suggesting this nice theorem and proof.

- One consequence of the Representer theorem only applies if $J(w)$ has a minimizer over $\mathcal{H}$. This theorem tells us that it's sufficient to check for a constrained minimizer of $J(w)$ over M. If one exists, then it's also an unconstrained minimizer of $J(w)$ over $\mathcal{H}$. If there is no constrained minimizer over M, then $J(w)$ has no minimizer over $\mathcal{H}$ (by the Representer theorem).
- Bottom Line: We can jump straight to minimizing over M, the "span of the data".

Sufficient Condition for Existence of a Minimizer (Proof)

1. Let $w_M^* \in \arg\min_{w \in M} J(w)$. [the constrained minimizer]
2. Consider any $w \in \mathcal{H}$.
3. Let $w_M = \text{Proj}_M w$.
4. By the Representer theorem, $J(w_M) \leqslant J(w)$.
5. $J(w_M^*) \leqslant J(w_M)$ by definition of w_M^*.
6. Thus for any $w \in \mathcal{H}$, $J(w_M^*) \leqslant J(w)$.
7. Therefore w_M^* minimizes $J(w)$ over $\mathcal{H}$

QED

Reparameterizing our Generalized Objective Function

Rewriting the Objective Function

- Define the training score function $s:\mathbf{R}^d \to \mathbf{R}^n$ by

$$s(w) = \begin{pmatrix} \langle w, x_1 \rangle \\ \vdots \\ \langle w, x_n \rangle \end{pmatrix},$$

  which gives the **training score vector** for any w.

- We can then rewrite the objective function as

$$J(w) = R(\|w\|) + L(s(w)),$$

  where now $L:\mathbf{R}^{n\times 1} \to \mathbf{R}$ takes a column vector as input.

- This will allow us to have a slick reparameterized version...

Reparameterize the Generalized Objective

- By the Representer Theorem, it's sufficient to minimize $J(w)$ for w of the form $\sum_{i=1}^{n} \alpha_i x_i$.
- Plugging this form into $J(w)$, we see we can just minimize

$$J_0(\alpha) = R\left(\left\|\sum_{i=1}^{n} \alpha_i x_i\right\|\right) + L\left(s\left(\sum_{i=1}^{n} \alpha_i x_i\right)\right)$$

  over $\alpha = (\alpha_1, \ldots, \alpha_n)^T \in \mathbf{R}^{n \times 1}$.

- With some new notation, we can substantially simplify
  - the norm piece $\|w\| = \|\sum_{i=1}^{n} \alpha_i x_i\|$, and
  - the score piece $s(w) = s\left(\sum_{i=1}^{n} \alpha_i x_i\right)$.

Simplifying the Reparameterized Norm

- For the norm piece $\|w\| = \|\sum_{i=1}^{n} \alpha_i x_i\|$, we have

$$
\begin{aligned}
\|w\|^2 &= \langle w, w \rangle \\
&= \left\langle \sum_{i=1}^{n} \alpha_i x_i, \sum_{j=1}^{n} \alpha_j x_j \right\rangle \\
&= \sum_{i,j=1}^{n} \alpha_i \alpha_j \langle x_i, x_j \rangle .
\end{aligned}
$$

- This expression involves the n^2 inner products between all pairs of input vectors.
- We often put those values together into a matrix...

The Gram Matrix

Definition

The **Gram matrix** of a set of points $x_1, \dots, x_n$ in an inner product space is defined as

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

- This is the traditional definition from linear algebra.
- Later today we'll introduce the notion of a "kernel matrix"
    - The Gram matrix is a special case of a **kernel matrix** for the identity feature map.
    - That's why we write K for the Gram matrix instead of G, as done elsewhere.
- NOTE: In ML, we often use Gram matrix and kernel matrix to mean the same thing. Don't get too hung up on the definitions.

Example: Gram Matrix for the Dot Product

- Consider $x_1,\ldots,x_n \in \mathbf{R}^{d\times 1}$ with the standard inner product $\langle x,x'\rangle = x^T x'$.
- Let $X \in \mathbf{R}^{n\times d}$ be the **design matrix**, which has each input vector as a row:

$$X = \begin{pmatrix} -x_1^T- \\ \vdots \\ -x_n^T- \end{pmatrix}.$$

- Then the Gram matrix is

$$\begin{aligned} K &= \begin{pmatrix} x_1^T x_1 & \cdots & x_1^T x_n \\ \vdots & \ddots & \cdots \\ x_n^T x_1 & \cdots & x_n^T x_n \end{pmatrix} = \begin{pmatrix} -x_1^T- \\ \vdots \\ -x_n^T- \end{pmatrix} \begin{pmatrix} | & \cdots & | \\ x_1 & \cdots & x_n \\ | & \cdots & | \end{pmatrix} \\ &= XX^T \end{aligned}$$

Simplifying the Reparametrized Norm

- With $w=\sum_{i=1}^{n}\alpha_i x_i$, we have

$$\begin{aligned}\|w\|^2 &= \langle w,w\rangle \\ &= \left\langle \sum_{i=1}^{n}\alpha_i x_i, \sum_{j=1}^{n}\alpha_j x_j \right\rangle \\ &= \sum_{i,j=1}^{n}\alpha_i\alpha_j \langle x_i,x_j\rangle \\ &= \alpha^T K\alpha.\end{aligned}$$

Simplifying the Training Score Vector

- The score for x_j for $w = \sum_{i=1}^{n} \alpha_i x_i$ is

$$\langle w, x_j \rangle \;=\; \left\langle \sum_{i=1}^{n} \alpha_i x_i, x_j \right\rangle = \sum_{i=1}^{n} \alpha_i \langle x_i, x_j \rangle$$

- The training score vector is

$$\begin{aligned}
s\left(\sum_{i=1}^{n} \alpha_i x_i\right) &= \begin{pmatrix} \sum_{i=1}^{n} \alpha_i \langle x_i, x_1 \rangle \\ \vdots \\ \sum_{i=1}^{n} \alpha_i \langle x_i, x_n \rangle \end{pmatrix} = \begin{pmatrix} \alpha_1 \langle x_1, x_1 \rangle + \cdots + \alpha_n \langle x_n, x_1 \rangle \\ \vdots \\ \alpha_1 \langle x_1, x_n \rangle + \cdots + \alpha_n \langle x_n, x_n \rangle \end{pmatrix} \\
&= \begin{pmatrix} \langle x_1, x_1 \rangle & \cdots & \langle x_1, x_n \rangle \\ \vdots & \ddots & \cdots \\ \langle x_n, x_1 \rangle & \cdots & \langle x_n, x_n \rangle \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} \\
&= K\alpha
\end{aligned}$$

Reparameterized Objective

- Putting it all together, our reparameterized objective function can be written as

$$\begin{aligned} J_0(\alpha) &= R\left(\left\|\sum_{i=1}^{n}\alpha_i x_i\right\|\right) + L\left(s\left(\sum_{i=1}^{n}\alpha_i x_i\right)\right) \\ &= R\left(\sqrt{\alpha^T K \alpha}\right) + L(K\alpha), \end{aligned}$$

  which we minimize over $\alpha \in \mathbf{R}^n$.
- **All information** needed about $x_1, \ldots, x_n$ is summarized in the Gram matrix K.
- We're now minimizing over $\mathbf{R}^n$ rather than $\mathbf{R}^d$.
- If $d \gg n$, this can be a big win computationally (at least once K is computed).

Reparameterizing Predictions

- Suppose we've found

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

- Then we know $w^* = \sum_{i=1}^n \alpha^* x_i$ is a solution to

$$\underset{w \in \mathcal{H}}{\arg\min}\, R(\|w\|) + L(\langle w, x_1 \rangle, \ldots, \langle w, x_n \rangle).$$

- The prediction on a new point $x \in \mathcal{H}$ is

$$\hat{f}(x) = \langle w^*, x \rangle = \sum_{i=1}^n \alpha_i^* \langle x_i, x \rangle.$$

- To make a new prediction, we may need to touch all the training inputs $x_1, \ldots, x_n$.

More Notation

- It will be convenient to define the following column vector for any $x \in \mathcal{H}$:

$$k_x = \begin{pmatrix} \langle x_1, x \rangle \\ \vdots \\ \langle x_n, x \rangle \end{pmatrix}$$

- Then we can write our predictions on a new point x as

$$\hat{f}(x) = k_x^T \alpha^*$$

Summary So Far

- Original plan:
  - Find $w^* \in \arg\min_{w\in\mathcal{H}} R\left(\|w\|\right) + L\left(\langle w, x_1\rangle, \ldots, \langle w, x_n\rangle\right)$
  - Predict with $\hat{f}(x) = \langle w^*, x\rangle$.
- We showed that the following is equivalent:
  - Find $\alpha^* \in \arg\min_{\alpha\in\mathbf{R}^n} R\left(\sqrt{\alpha^T K\alpha}\right) + L\left(K\alpha\right)$
  - Predict with $\hat{f}(x) = k_x^T\alpha^*$, where

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

  - 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

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

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

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

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

How to kernelize?

- Our principle tool for kernelization is reparameterization by the representer theorem.
- There are other methods – we used duality for SVM and bare hands for ridge regression.
- Below, we highlight key differences between
  - kernelized ridge regression and kernelized SVM at prediction time..

Kernel Ridge Regression

Kernelizing Ridge Regression

- Ridge Regression:

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \|Xw - y\|^2 + \lambda \|w\|^2$$

- Plugging in $w = \sum_{i=1}^{n} \alpha_i x_i$, we get the kernelized ridge regression objective function:

$$\min_{\alpha \in \mathbf{R}^n} \frac{1}{n} \|K\alpha - y\|^2 + \lambda \alpha^T K \alpha$$

- This is usually just called **kernel ridge regression**.

Kernel Ridge Regression Solutions

- For $\lambda > 0$, the **ridge regression solution** is

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

- and the **kernel ridge regression solution** is

$$\begin{aligned} \alpha^* &= (XX^T + \lambda I)^{-1} y \\ &= (K + \lambda I)^{-1} y \end{aligned}$$

- (Shown in homework.)
- For ridge regression we're dealing with a $d \times d$ matrix.
- For kernel ridge regression we're dealing an $n \times n$ matix.

Predictions

- Predictions in terms of w^*:
$$\hat{f}(x) = x^T w^*$$

- Predictions in terms of α^*:
$$\hat{f}(x) = k_x^T \alpha^* = \sum_{i=1}^{n} \alpha_i^* x_i^T x$$

- For kernel ridge regression, need to access all training inputs $x_1, \ldots, x_n$ to predict.
- For SVM, we may not...

Kernel SVM

Kernelized SVM (From Representer Theorem)

- The SVM objective:

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

- Plugging in $w = \sum_{i=1}^{n} \alpha_i x_i$, we get

$$\min_{\alpha \in \mathbf{R}^n} \frac{1}{2}\alpha^T K \alpha + \frac{c}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i \left(K\alpha\right)_i\right)$$

- Predictions with

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

- This is one way to kernelize SVM...

Kernelized SVM (From Lagrangian Duality)

- Kernelized SVM from computing the Lagrangian Dual Problem:

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

- If α^* is an optimal value, then

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

- 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

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

- 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**.

Are we done yet?

- Suppose our feature space is $\mathcal{H} = \mathbf{R}^d$.
- And we use representer theorem to kernelize.
- Get optimization problem over $\mathbf{R}^n$ rather than over $\mathbf{R}^d$:

$$\begin{aligned} \text{[original] } w^* &= \operatorname*{arg\,min}_{w \in \mathbf{R}^d} R(\|w\|) + L(\langle w, x_1 \rangle, \ldots, \langle w, x_n \rangle) \\ \text{[kernelized] } \alpha^* &= \operatorname*{arg\,min}_{\alpha \in \mathbf{R}^n} R\left(\sqrt{\alpha^T K \alpha}\right) + L(K\alpha) \end{aligned}$$

- This seems like a good move if $d \gg n$.
- However, there is still a hidden dependence on d in the kernelized form – do you see it?

Computational considerations – we're not really done yet

- Get optimization problem over $\mathbf{R}^n$ rather than over $\mathbf{R}^d$:

$$
\begin{aligned}
\text{[original] } w^* &= \operatorname*{arg\,min}_{w \in \mathbf{R}^d} R\left(\|w\|\right) + L\left(\langle w, x_1\rangle, \ldots, \langle w, x_n\rangle\right) \\
\text{[kernelized] } \alpha^* &= \operatorname*{arg\,min}_{\alpha \in \mathbf{R}^n} R\left(\sqrt{\alpha^T K \alpha}\right) + L\left(K\alpha\right)
\end{aligned}
$$

- For the standard inner product, $K_{ij} = \langle x_i, x_j\rangle = x_i^T x_j$, where $x_i, x_j \in \mathbf{R}^d$.
- This is still $O(d)$, and can be too slow for huge feature spaces.
- The essence of the "**kernel trick**" is getting around this $O(d)$ dependence.