Recap for Midterm

David S. Rosenberg

New York University

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Contents

Learning Theory Framework

Some Formalization

The Spaces

- $\mathcal{X}$: input space
- $\mathcal{Y}$: outcome space
- $\mathcal{A}$: action space

Prediction Function (or "decision function")

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

$$\begin{aligned} f: \quad \mathcal{X} &\to \mathcal{A} \\ x &\mapsto f(x) \end{aligned}$$

Loss Function

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

$$\begin{aligned} \ell: \quad \mathcal{A} \times \mathcal{Y} &\to \mathbf{R} \\ (a, y) &\mapsto \ell(a, y) \end{aligned}$$

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 exampe (x, y) drawn randomly from $P_{\mathcal{X}\times\mathcal{Y}}$.

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 $\mathcal{X}$ to $\mathcal{A}$.

- The risk of a Bayes prediction function is called the **Bayes risk**.

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

$$\hat{f} \in \arg\min_{f} \hat{R}_n(f),$$

  where the minimum is taken over all functions.

- But unconstrained ERM can **overfit**.

Constrained Empirical Risk Minimization

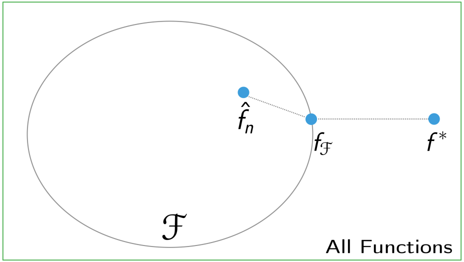
- Hypothesis space $\mathcal{F}$, a set of [prediction] functions mapping $\mathcal{X} \to \mathcal{A}$
- **Empirical risk minimizer** (ERM) in $\mathcal{F}$ is

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

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

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

Error Decomposition



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

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

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

- **Approximation Error** (of $\mathcal{F}$) $= \; R(f_{\mathcal{F}}) - R(f^*)$
- **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:

$$
\begin{aligned}
\textbf{Excess Risk}(\hat{f}_n) &= R(\hat{f}_n) - R(f^*) \\
&= \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}.
\end{aligned}
$$

Optimization Error

- In practice, we don't find the ERM $\hat{f}_n \in \mathcal{F}$.
- Optimization algorithm returns $\tilde{f}_n \in \mathcal{F}$, 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

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

- Extended decomposition:

$$\begin{aligned}
\textbf{Excess Risk}(\tilde{f}_n) &= R(\tilde{f}_n) - R(f^*) \\
&= \underbrace{R(\tilde{f}_n) - R(\hat{f}_n)}_{\text{optimization error}} + \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}
\end{aligned}$$

Regularization

Constrained Empirical Risk Minimization

Constrained ERM (Ivanov regularization)

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

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

$$\text{s.t. } \Omega(f) \leqslant r$$

- 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

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

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 $r \geqslant 0$ is

$$\hat{w} = \underset{\|w\|_2^2 \leqslant r^2}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2.$$

Lasso Regression: Workhorse (2) of Modern Data Science

Lasso Regression (Tikhonov Form)

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

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

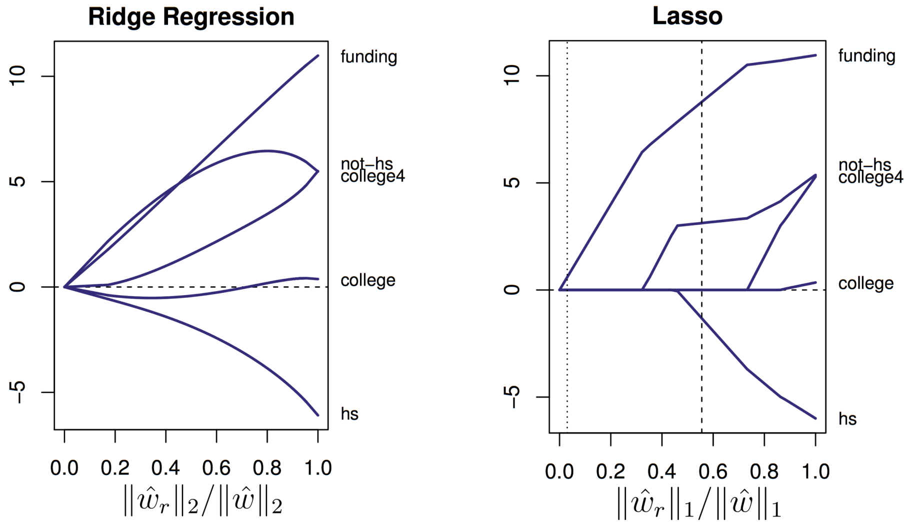
where $\|w\|_1 = |w_1| + \cdots + |w_d|$ is the ℓ_1-norm.

Lasso Regression (Ivanov Form)

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

$$\hat{w} = \operatorname*{arg\,min}_{\|w\|_1 \leqslant r} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2.$$

Ridge vs. Lasso: Regularization Paths

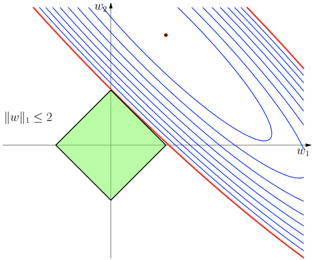


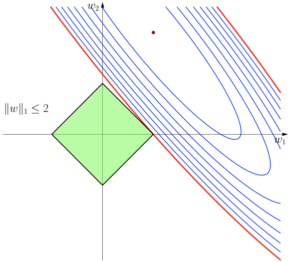
Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.

Linearly Dependent Features: Take Away

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

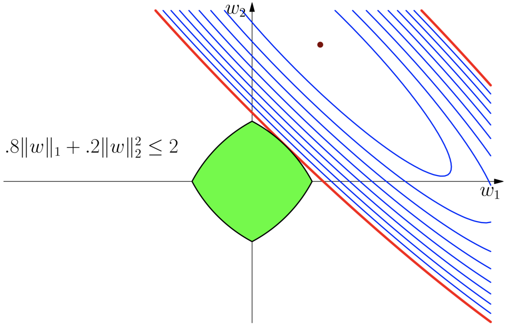
Elastic Net

- The **elastic net** combines lasso and ridge penalties:

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

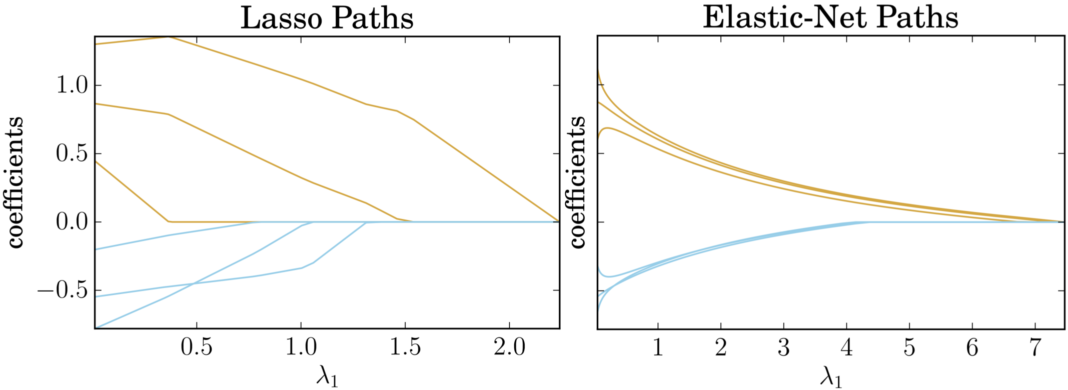
- We expect correlated random variables to have similar coefficients.

Highly Correlated Features, Elastic Net Constraint



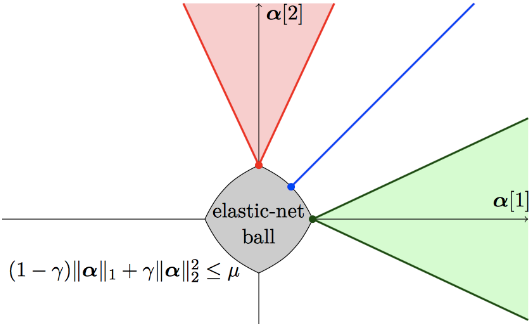
- Elastic net solution is closer to $w_2 = w_1$ line, despite high correlation.

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 - "Sparse Regions"



- Suppose design matrix X is orthogonal, so $X^T X = I$, and contours are circles (and features uncorrelated)
- Then OLS solution in green or red regions implies elastic-net constrained solution will be at corner

Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.9

Elastic Net Summary

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

Finding Lasso Solution

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

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

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

Optimization

Gradient Descent for Empirical Risk and Averages

- Suppose we have a hypothesis space of functions $\mathcal{F} = \left\{ f_w : \mathcal{X} \to \mathcal{A} \mid w \in \mathbf{R}^d \right\}$
  - Parameterized by $w \in \mathbf{R}^d$.
- 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 $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- 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
- Discussed in Concept Check question.

Descent Directions

- A step direction is a **descent direction** if, for small enough step size, the objective function value always decreases.
- Negative gradient is a descent direction.
- A negative subgradient is **not** a descent direction. But always **takes you closer to a minimizer**.
- Negative stochastic or minibatch gradient direction is **not** a descent direction. But we have convergence theorems.
- Negative stochastic subgradient step direction is **not** a descent direction. But we have convergence theorems (not discussed in class).

Classification

The Score Function

- Action space $\mathcal{A} = \mathbf{R}$ Output space $\mathcal{Y} = \{-1, 1\}$
- **Real-valued prediction function $f : \mathcal{X} \to \mathbf{R}$**

Definition

The value $f(x)$ is called the **score** for the input x.

- In this context, f may be called a **score function**.
- Intuitively, magnitude of the score represents the **confidence of our prediction**.

The Margin

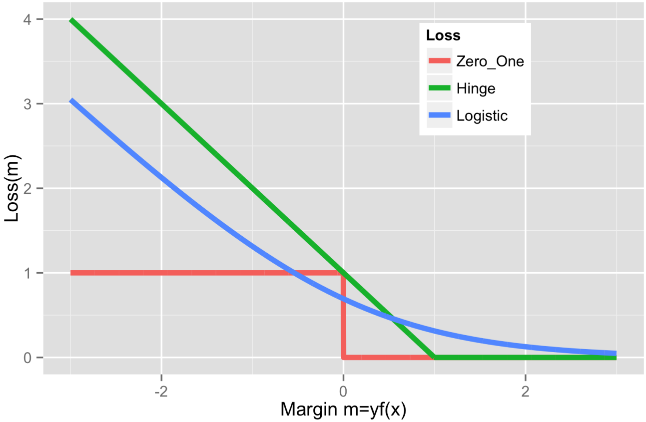
Definition

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 $f(x)$ is our score function.
- 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

Logistic/Log loss: $\ell_{\text{Logistic}} = \log\left(1+e^{-m}\right)$



Logistic loss is differentiable. Logistic loss always wants more margin (loss never 0).

Support Vector Machine

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

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

SVM as a Quadratic Program

- The SVM optimization problem is equivalent to

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

- 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.

The Representer Theorem and Kernelization

General Objective Function for Linear Hypothesis Space (Details)

- **Generalized objective**:

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

  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**).

- 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 $w = \operatorname{Proj}_M w^*$, for some minimizer w^* of $J(w)$.
- Then $\langle w, x_i\rangle = \langle w^*, x_i\rangle$, so loss part doesn't change.
- $\|w\| \leqslant \|w^*\|$, since projection reduces norm. So regularization piece never increases.

Reparametrization with Representer Theorem

- 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 $\hat{f}(x) = \langle w^*, x \rangle$.
- Plugging in result of representer theorem, it's equivalent to
  - 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

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

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

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

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

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

Kernelization

- Once we have kernelized:
  - $\alpha^* \in \arg\min_{\alpha \in \mathbf{R}^n} R\left(\sqrt{\alpha^T K \alpha}\right) + L(K\alpha)$
  - $\hat{f}(x) = k_x^T \alpha^*$
- 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:

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

- 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**.