Review for Midterm

DS-GA 1003 Machine Learning

NYU CDS

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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 example (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:

$$f^* \in \arg\min_f R(f),$$

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**.

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 $f^*(x) = \underset{c \in \mathcal{Y}}{argmax}\ p(y = c|x)$

Question: Let x be sampled uniformly from $\{-100, -99, \ldots, 99, 100\}$. 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 $\mathcal{D}_n = ((x_1, y_1), \ldots, (x_n, y_n))$ 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

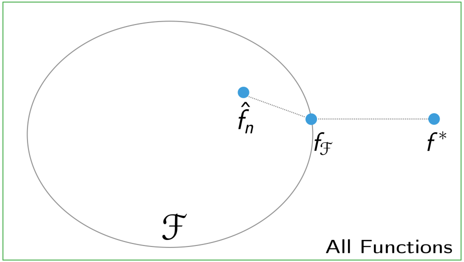
- Hypothesis space $\mathcal{F}$, a set of [prediction] functions mapping $\mathcal{X} \to \mathcal{A}$
- **Empirical risk minimizer** (ERM) in $\mathcal{F}$ is

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

- **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:

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

Question

Select true of false for each of the following statements:

1. Approximation Error is a Random Variable
2. Estimation Error is a Random Variable
3. Optimization Error is a Random Variable.
4. If the hypothesis space consists of all possible functions, then approximation error is non-zero.
5. Estimation Error can be negative.
6. Optimization Error can be negative.
7. 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 $\leqslant$, $\geqslant$, 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.

1. 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.
4. 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.
3. The empirical risk of f_1 will be larger.
4. 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.
5. Cannot be determined.

Regularization

Constrained Empirical Risk Minimization

Constrained ERM (Ivanov regularization)

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

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

- 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

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

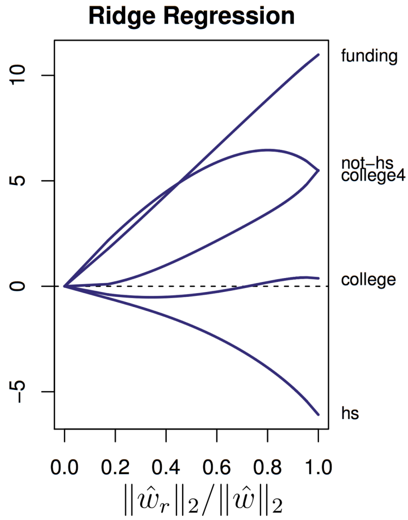
where $\|w\|_1 = |w_1| + \cdots + |w_d|$ is the ℓ_1-norm.

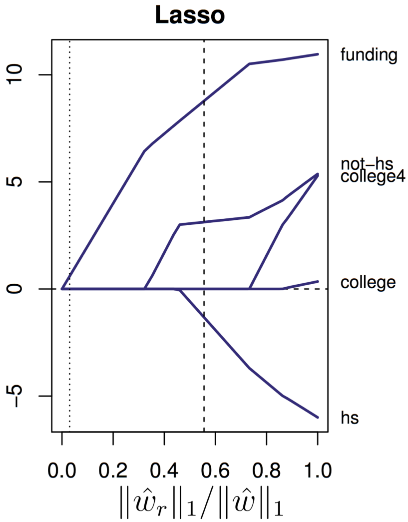
Lasso Regression (Ivanov Form)

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

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

Ridge vs. Lasso: Regularization Paths



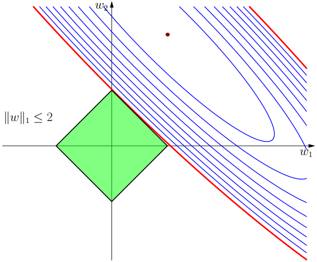


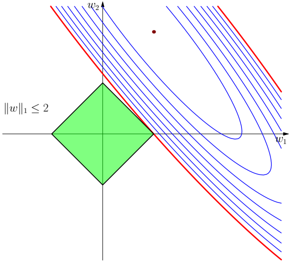
Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.

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?)

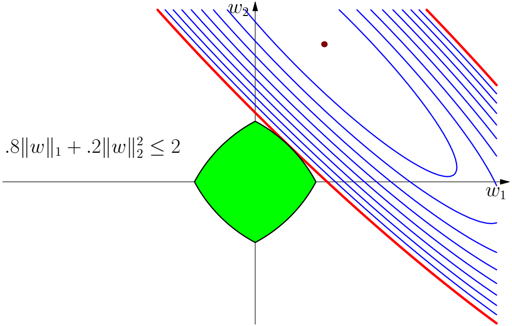
Elastic Net

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

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

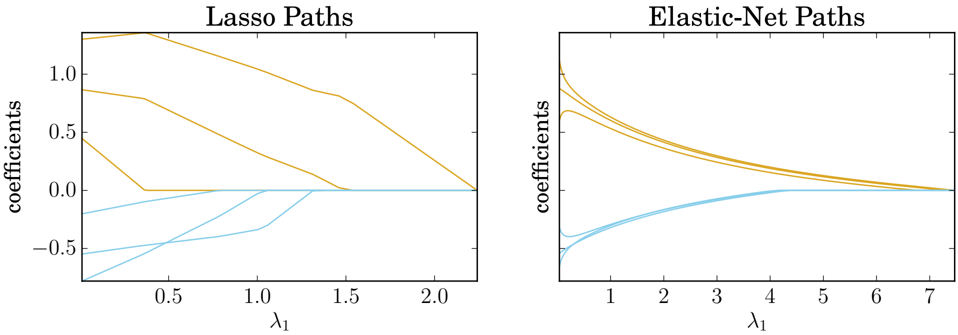
- We expect correlated random variables to have similar coefficients.

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 $\mathcal{R}^4$. 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:

1. $(0, 1.2, 6.7, 2.1)^T$
2. $(0.6, 0.6, 6.7, 2.1)^T$
3. $(1.2, 0, 6.7, 2.1)^T$
4. $(-0.1, 1.3, 6.7, 2.1)^T$

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

$$\min_{w^+,w^-} \quad \sum_{i=1}^{n}\left(\left(w^+ - w^-\right)^T x_i - y_i\right)^2 + \lambda 1^T\left(w^+ + w^-\right)$$

$$\text{subject to} \quad w_i^+ \geqslant 0 \text{ for all } i \qquad w_i^- \geqslant 0 \text{ for all } i,$$

- 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 $\mathcal{F} = \left\{ f_w : \mathcal{X} \to \mathcal{A} \mid w \in \mathbf{R}^d \right\}$
  - 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

Subgradient Review

Definition (Subgradient and Subdifferential)

A vector g is a subgradient of (convex) $f : \mathcal{R}^d \to \mathcal{R}$ at x if for all z

$$f(z) \geqslant f(x) + g^T(z - x)$$

. The set of all subgradients at x is called the subdifferential of f at x $\partial f(x)$

Questions:

1. (True/False) If f is convex and differentiable everywhere in the domain, then $\partial f(x) = \{\nabla f(x)\}$
2. (True/False) The subdifferential of f at x, $\partial f(x)$ is always a convex set. (Null set is trivially complex)

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).

Decide whether the following statements apply to full batch gradient descent (GD), mini- batch GD, neither, or both.

Assume we're minimizing a differentiable, convex objective function $J(w) = \frac{1}{n}\sum_{i=1}^{n} f_i(w)$, and we are currently at w_t, which is not a minimum. For full batch GD, take $v = \nabla_w J(w_t)$, and for minibatch GD take v to be a minibatch estimate of $\nabla_w J(w_t)$ based on a random sample of the training data.

1. For any step size $\eta > 0$, after applying the update rule $w_{t+1} \leftarrow w_{tl} - \eta v$. we must have $J(w_{t+1}) < J(w_t)$.
2. There must exist some $\eta > 0$ such that after applying the update rule $w_{t+1} + w_t - \eta v$ we have $J(w_{t+1}) < J(w_t)$.
3. v is an unbiased estimator of the full batch gradient.

Classification

The Score Function

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

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

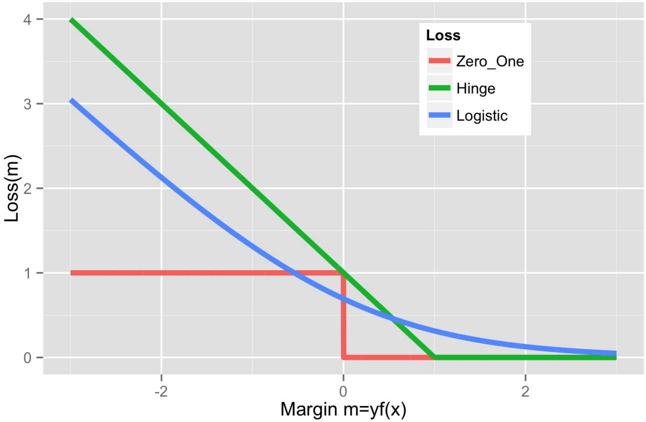
Definition

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

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

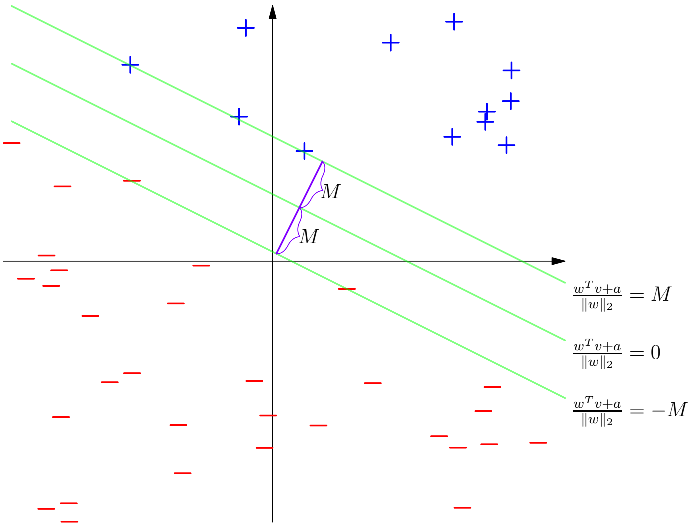
- Differentiable objective function
- $n + d + 1$ unknowns and $2n$ affine constraints.
- A quadratic program that can be solved by any off-the-shelf QP solver.
- We arrived at this optimization problem also from a geometric prospective.

Linear Separability and Hard Margin SVM

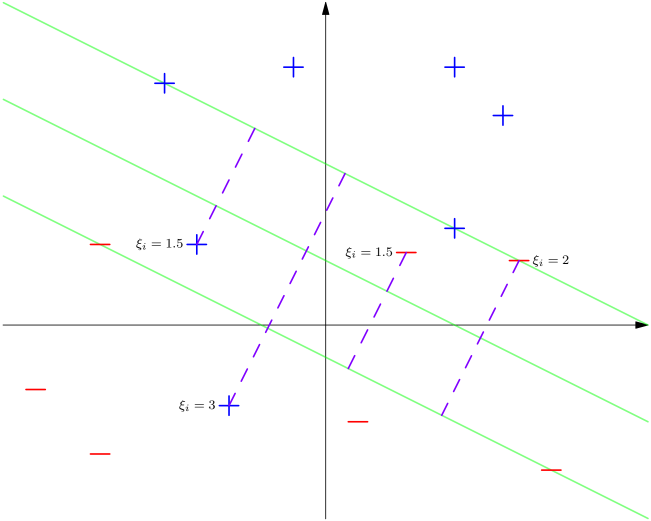
Definition (Linear Separability)

We say (x_i, y_i) for $i = 1, \ldots, n$ are *linearly separable* if there is a $w \in \mathcal{R}^d$ and $b \in \mathcal{R}$ such that $y_i(w^T x_i - b) > 0$ for all i. The set $\{v \in \mathcal{R}^d \mid w^T v - b = 0\}$ is called a *separating hyperplane*.

Maximum Margin Separating Hyperplane



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



Question on Classification

Suppose $x_1, \ldots, x_n \in \mathbb{R}^d$ and $y_1, \ldots, y_n \in \{-1, 1\}$. Here we look at y_i as the label of x_i. We say the data points are linearly separable if there is a vector $v \in \mathbb{R}^d$ and $a \in \mathbb{R}$ such that $v^T x_i > a$ when $y_i = 1$ and $v^T x_i < a$ for $y_i = -1$. Give a method for determining if the given data points are linearly separable.

The Representer Theorem and Kernelization

General Objective Function for Linear Hypothesis Space (Details)

- **Generalized objective**:

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

  where

  - $w, x_1, \ldots, x_n \in \mathcal{H}$ for some Hilbert space $\mathcal{H}$. (We typically have $\mathcal{H} = \mathbb{R}^d$.)
  - $\|\cdot\|$ is the norm corresponding to the inner product of $\mathcal{H}$. (i.e. $\|w\| = \sqrt{\langle w, w\rangle}$)
  - $R : [0, \infty) \to \mathbb{R}$ 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 $J(w) = R\left(\|w\|\right) + L\left(\langle w, x_1\rangle, \ldots, \langle w, x_n\rangle\right)$ 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 $M = \operatorname{span}\left(x_1, \ldots, x_n\right)$. [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 $w^* \in \arg\min_{w \in \mathcal{H}} R(\|w\|) + L(\langle w, x_1 \rangle, \ldots, \langle w, x_n \rangle)$
  - Predict with $\hat{f}(x) = \langle w^*, x \rangle$.
- Plugging in result of representer theorem, it's equivalent to
  - Find $\alpha^* \in \arg\min_{\alpha \in \mathbb{R}^n} R\left(\sqrt{\alpha^T K \alpha}\right) + L(K\alpha)$
  - Predict with $\hat{f}(x) = k_x^T \alpha^*$, where

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

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

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

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

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

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

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

Kernelization

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

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

- 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

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

- 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**.

Question on Kernel

Consider the objective function

$$J(w) = \|Xw - y\|_1 + \lambda \|w\|_2^2$$

Assume we have a positive semidefinite kernel k.

1. What is the kernelized version of this objective?
2. Given a new test point x, find the predicted value.

MLE and Conditional Probability Models

Maximum Likelihood Estimation

- Suppose $\mathcal{D} = (y_1, \dots, y_n)$ is an i.i.d. sample from some distribution.

Definition

A **maximum likelihood estimator (MLE)** for θ in the **parametric model** $\{p(y;\theta) \mid \theta \in \Theta\}$ is

$$\begin{aligned} \hat{\theta} &\in \underset{\theta \in \Theta}{\arg\max} \log p(\mathcal{D}, \hat{\theta}) \\ &= \underset{\theta \in \Theta}{\arg\max} \sum_{i=1}^{n} \log p(y_i;\theta). \end{aligned}$$

Maximum Likelihood Estimation

- Finding the MLE is an **optimization problem**.
- For some model families, calculus gives a closed form for the MLE.
- Can also use numerical methods we know (e.g. SGD).

Conditional Distribution Estimation (Generalized Regression)

- Task: Given x, predict probability distribution $p(y|x)$
- Method:
  1. Represent $p(y|x)$ with *parametric families* of distributions: $p(y;\theta(x))$ with parameters θ.
  2. Maximize likelihood of training data: $\hat{\theta} \in \arg\max_{\theta} \log p(\mathcal{D}, \hat{\theta})$
- Models covered:
  1. Logistic regression (Bernoulli distribution)
  2. Poisson regression (Poisson distribution)
  3. Conditional Gaussian/Linear regression (Normal distribution, fixed variance)
  4. Multinomial Logistic Regression (Multinoulli/Categorical distribution)

Linear Probabilistic Classifiers

- Setting: $\mathcal{X} = \mathbf{R}^d$, $\mathcal{Y}$ arbitrary for now
- Want prediction function to map each $x \in \mathbf{R}^d$ to $\theta \in \Theta$ for $p(y; \theta(x))$.
- For a **linear method**, we first **extract information** from $x \in \mathbf{R}^d$ and summarize in a single number with a linear function:

$$\underbrace{x}_{\in \mathbf{R}^d} \mapsto \underbrace{w^T x}_{\in \mathbf{R}}$$

  (That number is analogous to the **score** in classification.)
- As usual, $x \mapsto w^T x$ will include affine functions if we include a constant feature in x.
- $w^T x$ is called the **linear predictor.**
- Still need to map this to Θ.

The Transfer Function

- Need a function to map the linear predictor in R to Θ:

$$\underbrace{x}_{\in \mathbb{R}^d} \mapsto \underbrace{w^T x}_{\in \mathbb{R}} \mapsto \underbrace{f(w^T x)}_{\in \Theta} = \theta,$$

  where $f : \mathbb{R} \to \Theta$. We'll call f the **transfer** function.

- So prediction function is $x \mapsto f(w^T x)$.
- The prediction function gives us the parameter for $p(y; \theta(x))$ used to estimate $p(y|x)$.

Conditional Probability Modeling as Statistical Learning

- Input space $\mathcal{X}$
- Outcome space $\mathcal{Y}$
- All pairs (x, y) are independent with distribution $P_{\mathcal{X}\times\mathcal{Y}}$.
- **Action space** $\mathcal{A} = \{p(y) \mid p$ is a probability density or mass function on $\mathcal{Y}\}$.
- Hypothesis space $\mathcal{F}$ contains decision functions $f : \mathcal{X} \to \mathcal{A}$.
- Maximum likelihood estimation for dataset $\mathcal{D} = ((x_1, y_1), \ldots, (x_n, y_n))$ is

$$\hat{f}_{\text{MLE}} \in \underset{f \in \mathcal{F}}{\arg\max} \sum_{i=1}^{n} \log\left[f(x_i)(y_i)\right]$$

Conditional Probability Modeling as Statistical Learning

- Take loss $\ell : \mathcal{A} \times \mathcal{Y} \to R$ for a predicted PDF or PMF $p(y)$ and outcome y to be

$$\ell(p, y) = -\log p(y)$$

- The risk of decision function $f : \mathcal{X} \to \mathcal{A}$ is

$$R(f) = -\mathbb{E}_{x,y} \log \left[f(x)(y) \right],$$

where $f(x)$ is a PDF or PMF on $\mathcal{Y}$, and we're evaluating it on y.

- The empirical risk of f for a sample $\mathcal{D} = \{y_1, \ldots, y_n\} \in \mathcal{Y}$ is

$$\hat{R}(f) = -\frac{1}{n}\sum_{i=1}^{n} \log\left[f(x_i)(y_i)\right].$$

  This is called the negative **conditional log-likelihood**.
- Thus for the negative log-likelihood loss, ERM and MLE are equivalent

Question on Maximum Likelihood Estimation

1. Suppose we have samples $x_1, \ldots, x_n$ i.i.d. drawn from uniform distribution $\mathcal{U}(-a, a)$. Find the maximum likelihood estimator of a.
2. Which of the following models can be learned by MLE?
    - Perceptron
    - Logistic regression
    - SVM

References

- DS-GA 1003 Machine Learning Spring 2019
- DS-GA 1003 Machine Learning Spring 2020