Foundations of Machine Learning (CS5590)

Instructor: Saketh

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Lecture 1

Definition and Motivation

1. We noted an informal definition of Machine Learning as "The grand goal in ML is to develop computer programs that can mimic high-level cognitive abilities in humans for solving complex problems (e.g., those in Astrophysics, Biology, Environment etc.)".

2. The key challenge and uniqueness in developing such programs is that we are far from even roughly understanding how humans accomplish high-level cognitive tasks like concept acquisition, systematic decision making, evaluative and creative thinking, abstraction and summarization etc. Hence the idea is not to replicate human intelligence but to merely mimic the accomplishment of these tasks to near human performance level. This then coupled with the usual efficiencies of computers, may hopefully lead to solving complex problems that are currently beyond the reach of human intelligence. Read also section 1.2 in Shalev-Shwartz and Ben-David [2014].

3. We noted an important characteristic of human learning that we also hence desire for machine learning programs: it is not that human learning is error-free, neither is it that it is always near-accurate. The fact is that it is near-accurate most of the times. And as experience increases (i.e., as human learns), both the frequency of the number of times they err (beyond a threshold), and the worst case error in a given (yet high) fraction of evaluations, decrease.

4. Another important clarification we noted was the fact that it is the bias in humans (like "intuition" or "thoughts that come") that forms the basis for learning. Given the same experience, some humans may have the right bias for accomplishing a task well; whereas some others may not. Though both are indeed cases of human learning, the goal in ML is to mimic the

former i.e., develop models that have the right bias. This is nicely explained in section 1.1 in Shalev-Shwartz and Ben-David [2014] with the rats and pigeons example (we want to mimic learning in rats and not that in pigeons :).

5. Read section 1.4 in Shalev-Shwartz and Ben-David [2014] to understand the relation between ML and other fields like Statistics etc.

Lecture 2

Example Pipeline (stages) in ML

We noted an example pipeline in ML (somewhat a typical one though; but far from a universal one):

1. Story begins with an underlying concept. For example, the complex relationship between diseases and symptoms.
2. So called training data is collected that is a collection of records that implicitly/explicitly represent various instantiations/invokings of the concept. For example, each datum is a pair of medical record and corresponding disease diagnosis by an expert doctor.
3. Core ML stages:
   (a) Pick/design a model with right bias. For example restrict the search to relevant/known correlations or exclude some implausibilities or assume forms for underlying distributions etc. Given the model, learning is typically posed as a stochastic optimization problem (SOP).
   (b) Solve the SOP using the training data (this stage is typically dubbed as learning/training):
      i. development of learning algorithm
      ii. development of corresponding code
   (c) Use the solution of the SOP to build an inference machine that can deploy the skill acquired (concept learned). For example, the inference machine must take input as a new patient's record and conclude if he has a particular disease.
4. The model and learning algorithm must be theoretically analyzed to provide guarantees on performance improvement with training data size.

5. Scale the above for solving complex problems. For e.g., ML may only solve a part of the complex problem or one may redo some/all of the above steps in case of unacceptably low performance etc.

6. Deploy the inference machine in real-world. For e.g., handle adversaries, privacy concerns, ethics, law etc.

We noted that success at every stage is crucial. We only focus on 3(a)-3(c) in this course. Step 4 is subject of discussion in statistical learning theory courses. Mainstream ML research mainly focuses on issues in 3-4.

We then emphasized on the importance/convenience of making distributional assumptions in context of ML[1]:

1. Once such assumptions are made on the data, for e.g., data is a set of iid samples from a fixed (but unknown) distribution, then by law of large numbers kind of arguments, it is clear that the estimates (like sample mean) become "better" as number of samples increases. This naturally gives us a way of mimicking human learning which becomes "better" with experience (data).

2. It is easy to take into account uncertainties in data (measurement errors or unknown/unmeasured factors etc.).

[1] We also gave some coin tossing based learning concepts as examples.

Lecture 3

Supervised Learning

We begin with a very simple set-up for learning (refer section 2.1 and 1,2 paras in section 3.2.1 in Shalev-Shwartz and Ben-David [2014]):

1. It is assumed that the underlying concept (unknown yet fixed) is assumed to be a joint distribution between so called inputs/data-points and outputs/labels. More specifically, we assume that there exists a probability distribution (probability measure) P^* over $\mathcal{X}, \mathcal{Y}$, where $\mathcal{X}$ and $\mathcal{Y}$ are the sets of inputs and outputs respectively. We denote by p^* the corresponding likelihood[1] function for P^*.

2. It is assumed a set of m iid samples from p^* are given, called the training set. Intuitively, training set is intended to be used to explicitly/implicitly learn the underlying concept. We denote this training set by $\mathcal{D} \equiv \{(x_1, y_1), \ldots, (x_m, y_m)\}$, where $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ denotes the i^{th} independent sample from p^*.

3. It is assumed that a loss function $l : \mathcal{Y} \times \mathcal{Y}$ is given that quantifies the mismatch between any pair of outputs.

4. If $\mathcal{Y}$ is a discrete set with no[2] known relations between its elements, then the Supervised learning problem is known as Classification problem. An example loss function in this case is the so-called 0-1 loss: $l_{01}(a, b) \equiv \begin{cases} 0 & \text{if } a = b \\ 1 & \text{if } a \neq b \end{cases}$.

[1] i.e., p^* is the (joint) probability mass function if the distribution is (jointly) discrete, it is the (joint) probability density function if the distribution is (jointly) continuous, it is given by $p^*(x, y) \equiv p^*(x/y)p^*(y) = p^*(y/x)p^*(x)$ if one of the marginals is continuous and the other is discrete etc.

[2] If it is discrete set with a known total order that exists, then the supervised learning problem is known as an Ordinal Regression problem etc.

Further, if $|\mathcal{Y}| = 2$, then we qualify such a classification problem as a binary classification problem. The elements of $\mathcal{Y}$ are known as "classes".

5. If $\mathcal{Y}$ is an uncountable subset of reals, then the Supervised learning problem is qualified as a Regression problem. An example loss function in this case is the so-called squared loss: $l_2(a, b) \equiv (a - b)^2$. Refer section 3.2.2 in Shalev-Shwartz and Ben-David [2014].

6. Under these modeling assumptions, given the training data and the loss function, the ideal goal of Supervised learning is to find a function $g^* : \mathcal{X} \mapsto \mathcal{Y}$ such that

$$g^* \in \arg\min_g R[g], \text{ where } R[g] \equiv \mathbb{E}_{(X,Y)\sim P^*}\left[l\left(g\left(X\right), Y\right)\right]. \tag{3.1}$$

   $R[g]$, the expected loss, is also known as the Risk[3] with g. g^* is known as the Bayes optimal.

The above is the complete specification of a Supervised learning problem.

Note that the only information given for computing the Bayes optimal is the training set. Such optimization problems that minimize expectation under a distribution that is only known through its samples are called as Stochastic Optimization problems. In other words, in order to compute the Bayes optimal, one needs to solve the stochastic optimization problem of Risk minimization defined in (3.1).

There exists vastly different strategies to "solve" (3.1). Broadly, they can be categorized as Probabilistic modeling and non-probabilistic modeling. The subsequent discussion presents one particular framework that can be categorized under the later.

[3] $\mathbb{E}_{(X,Y)\sim P^*}\left[l\left(g\left(X\right), Y\right)\right]$ is given by $\int_{\mathcal{X}}\int_{\mathcal{Y}} l\left(g\left(x\right), y\right) \mathrm{d}P^*(x, y)$. For e.g., this evaluates to the usual sum formula involving pmf for discrete rvs and evaluates to the usual integral formula involving pdf for the conts case etc. It is also useful to recall the total expectation rule.

Lecture 4

Empirical Risk Minimization

One obvious idea is to perhaps approximate the expected loss with average loss computed over training set: $\min_g \frac{1}{m}\sum_{i=1}^{m} l(g(x_i), y_i)$. The motivation for this is the law of large numbers that guarantees that the average (loss with g) over the training set will be arbitrarily close to the expectation (of loss with g), with arbitrarily high probability, provided m is big enough! Please refer section 2.2.1 in Shalev-Shwartz and Ben-David [2014] too.

Though this is true for a given g, the minimization spoils the result. For e.g., one can trivially consider functions $\bar{g}$ such that $\bar{g}(x_i) \equiv y_i \ \forall \ i = 1, \ldots, m$. And elsewhere its value, $\bar{g}(x)$, is arbitrary. It is easy to see that such so-called memorization functions are guaranteed to minimize the average loss, but nevertheless may incur arbitrarily high (true) risk.

One way around is when we assume that it is known apriori that the Bayes optimal belongs to a particular class of functions, say $\mathcal{G}$, henceforth referred to as the inductive bias or Hypothesis class. For example, in the Ohm's law experiment from school days, one knows apriori that the Bayes optimal is a linear function. So in that regression problem, one may safely assume the so-called linear inductive bias (i.e., $\mathcal{G}$ is set of all linear functions over the input space). Under such a modeling assumption, it is not difficult to see that the (true) risk may not be arbitrarily high with the functions that minimize the so-called empirical risk, which is the average loss over the training set. Hence one resorts to solving the following Empirical risk minimization (ERM) problem with inductive bias:

$$\hat{g}_m(\mathcal{G}) \in \arg\min_{g \in \mathcal{G}} \frac{1}{m}\sum_{i=1}^{m} l\left(g\left(x_i\right), y_i\right). \tag{4.1}$$

The golden question now is how bad is the ERM (with inductive bias) so-

lution compared to the Bayes optimal? This is answered by the fundamental theorem 26.5(3) (and results like lemma 26.10) in your textbook Shalev-Shwartz and Ben-David [2014], which is summarized below using our notation:

Theorem 4.0.1. *With probability* $1-\delta$,

$$R[\hat{g}_m(\mathcal{G})] \leq R[g^*(\mathcal{G})] + O\left(\sqrt{\frac{\mathcal{C}(l \circ \mathcal{G})}{m}}, \sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{m}}\right),$$

where $g^*(\mathcal{G})$ *is a (true) risk minimizer among functions in* $\mathcal{G}$, *and* $\mathcal{C}(l \circ \mathcal{G})$ *is the "complexity/capacity"*[1] *of the loss-inductive-bias combination (henceforth referred to as the model). We define* $R[\hat{g}_m(\mathcal{G})] - R[g^*(\mathcal{G})]$ *as the estimation error.*

The key take-homes from the above theorem are:

1. Estimation error will be arbitrarily small, with arbitrarily high probability, provided m is large enough, and $\mathcal{C}(l \circ \mathcal{G})$ is finite. So in machine learning we always design models with finite capacity[2]! Theorem 6.6 in Shalev-Shwartz and Ben-David [2014] is one formal result that confirms that infinitely complex models don't learn.

2. Weaker the inductive bias, bigger is the respective model's complexity, and worse is the upper bound on the (true) risk with the ERM solution (again with high probability). In other words, bigger models are more likely[3] to worsen the estimation error. Also, roughly speaking, steeper/finer[4] the loss function, greater the complexity.

Now, it is indeed trivial to observe that $R[g^*(\mathcal{G})] = R[g^*]$ whenever $g^* \in \mathcal{G}$. However in some cases, there may be a modeling error in the sense that the Bayes optimal is not in $\mathcal{G}$ being employed. In such cases, the quantity $R[g^*(\mathcal{G})] - R[g^*]$, henceforth called as approximation/model error, is also crucial. We define generalization error as the sum of estimation and approximation errors and is equal to

[1] Actually this is a term related to formally defined Complexity/Capacity like VC-dimension/Rademacher etc.

[2] Please do not confuse finite capacity as finite cardinalty. There are many models that allow uncountably infinite members but have finite capacity. See for e.g., section 6.1 in Shalev-Shwartz and Ben-David [2014]

[3] It is very essential to understand that there is still some chance that small/tiny models also may have high estimation error! Secondly, there may be "easy" concepts where the bound is loose and hence even enormous models may have low estimation error!!

[4] Informally, if the loss changes greatly with the change in its inputs, then it is steeper/finer. If loss ignores/is-less-sensitive to variations in (some) inputs, then it is flat/coarser.

$R[\hat{g}_m(\mathcal{G})] - R[g^*]$. In other words, for learning to be successful we need the generalization error to be low, which in turn means model error as well as estimation error are low. This break-up of errors is explained in section 5.2 in Shalev-Shwartz and Ben-David [2014].

In cases where there is not even partial information available regarding the characteristics of the Bayes optimal, one faces the challenges of trading-off between a weak inductive bias, where, most likely, estimation error may be high, but model error is low, and a strong inductive bias, where, most likely, estimation error is low, however model error may be high.

In practice, if modeling assumes something that is not true in the real-world application, then the model is unnecessarily small leading to poor generalization mainly because model error is large. On the contrary, if modeling misses to assume something that is known to be satisfied in the application, then the model is unnecessarily large leading to poor generalization again, but now because estimation error is large. In the later scenario, it is popular to say that the prediction function, $\hat{g}$, is overfitting the training data. This terminology is because in such cases the empirical risk with $\hat{g}$ may be low whereas the (true) risk with $\hat{g}$ will be high. Refer section 2.2.1 in Shalev-Shwartz and Ben-David [2014]. Since the key artifact in ERM is the inductive bias set, whose elements are functions, such a framework for modeling falls under the category of non-probabilistic modeling. Later we shall introduce so-called probabilistic modeling techniques where the key aspect is modeling distributions. Such trade-offs are detailed in chapter 5 in Shalev-Shwartz and Ben-David [2014].

We then began giving examples of some named (non-probabilistic) models in case of regression and classification.

Lecture 5

ERM: Regression

The first example model for regression over $\mathcal{X} = \mathbb{R}^n, \mathcal{Y} = \mathbb{R}$ is that with linear inductive bias, $\mathcal{L} \equiv \left\{ g \mid \exists\ w \in \mathbb{R}^n \ni g(x) = w^\top x\ \forall\ x \in \mathcal{X} \right\}$, and square loss. This loss-inductive-bias combo is known as the Linear Regression model. The variables w are called as the parameters of the linear/linear-regression model.

Please refer section 9.2 in Shalev-Shwartz and Ben-David [2014] for details of linear regression. The ERM solutions turn out to be those of the Normal equation corresponding to the set of linear equations given by: $X^\top w = y$, where X is the matrix with columns as the training input vectors, and y has entries as the training labels. In the special case $XX^\top$ is invertible, ERM has a unique solution given by the left inverse of $X^\top$ (least square solution).

Linear regression is not well-suited for high dimensional settings (even when model error is zero), because the complexity of models with linear inductive bias typically grow adversely with the dimensionality. For example, so-called (pseudo) "growth function" with linear inductive bias[1] increases exponentially[2] with no. of dimensions. Consequently, $\mathcal{C}$ happens to grow almost linearly[3] with dimensionality for linear regression. So, on one hand one might want to consider all known covariates for estimating the outputs, whereas inherently that may lead to bad generalization because of increased estimation error! This is called the "curse of dimensionality". The adverse effect of the curse of dimensionality can be reduced to a certain extent if one employs the following inductive bias instead:

Norm-bounded linear functions $\mathcal{L}_W \equiv \left\{ g \mid \exists\ w \in \mathbb{R}^n, \|w\|_2 \leq W \ni g(x) = w^\top x\ \forall\ x \in \mathcal{X} \right\}$. It can be shown that its complexity (when composed with some standard loss func-

[1] Growth function intuitively captures the notion of largeness of a set.
[2] For e.g., last equation on page 341 in Shalev-Shwartz and Ben-David [2014].
[3] For e.g., second equation on page 342 in Shalev-Shwartz and Ben-David [2014].

tions) is proportional[4] to W, and more importantly, is independent of dimensions! This makes $\mathcal{L}_W$ especially attractive for high-dimensional problems. Note that there is one model for every W, hence-forth referred to as the hyper-parameter. In other words, ridge regression is a family of models "parameterized" by the hyper-parameter, W. Needless to say, the usual trade-off applies: as W increases then model error decreases while estimation error increases.

$\mathcal{L}_W$ together with square-loss is known as the Ridge regression model. Refer section 13.1.1 in Shalev-Shwartz and Ben-David [2014] for details. We said the equivalent, nevertheless more popular, form of writing the corresponding ERM problem is eqn. 13.3 in Shalev-Shwartz and Ben-David [2014][5]. In this equivalent (Tikhonov form), λ plays the role of hyper-parameter, known as "Ridge". We commented that the ERM solution in this form is unique, and in the case $\lambda \downarrow 0$, the solution corresponds to the psuedoinverse solution for the linear equations $X^\top w = y$. We commented that ridge regression has many other attractive properties other than generalization: i) always unique solution ii) numerical stable algorithms iii) stability. These are detailed in sections 13.2-13.3 in Shalev-Shwartz and Ben-David [2014].

The above discussion shows how ERM recovers known fundamental results from linear algebra. We end discussion on regression for now with yet another model, this time based on a different loss function.

Consider the ϵ-insensitive loss defined by: $l(a, b) \equiv \max(0, |a - b| - \epsilon)$. This loss together with $\mathcal{L}_W$ bias is called as Support Vector Regression model. Since this is a coarser loss function, it is expected to lead to lesser model complexity. Refer `https://alex.smola.org/papers/2003/SmoSch03b.pdf` for details of this model. The other advantages are i) Sparse solution (solution depends only on few datapoints lying outside the ϵ margin, called support vectors) ii) Efficient solvers etc.

[4] For e.g., refer lemma 26.10 in Shalev-Shwartz and Ben-David [2014].

[5] Refer `https://link.springer.com/article/10.1007/s10994-015-5540-x` for details of equivalent forms.

Lecture 6

ERM: Classification

We begin with the simple case of binary classification. Let 1 and -1 denote the two classes in the binary classification problem. One way of using real-valued functions (like linear ones) for binary classification is to consider sign $(g(x))$ as output rather than $g(x)$. An obvious modeling is to use signed linear functions (or Halfspaces) as the inductive bias along with the 0-1 loss. Refer section 9.1 in Shalev-Shwartz and Ben-David [2014] for details. The corresponding ERM turns out to be a computationally hard problem[1]. However, in the special case where the training data is linearly separable, i.e., $\exists w \ni y_i w^\top x_i \geq 0 \ \forall \ i = 1, \ldots, m$, it can either be posed as a Linear Program (section 9.1.1), or solved using the so-called Perceptron algorithm that converges in finite no. iterations (section 9.1.2). Again, for analogous reasons as in regression, halfspaces are plagued with the curse of dimensionality.

We hence plan to use the $\mathcal{L}_W$ model for controlling model complexity. Also, we generalize the notion of loss function to $l : \mathcal{X} \times \mathcal{Y} \times \mathcal{G} \mapsto \mathbb{R}$. We consider hinge-loss given by $l(x, y, w) \equiv \max(0, 1 - yw^\top x)$. The combination of $\mathcal{L}_W$ and hinge-loss is called as the Support Vector Machine (SVM) model, whose ERM is given by eqn. 15.4 in Shalev-Shwartz and Ben-David [2014]. Please refer chapter 15 more details. We discussed how SVMs implement the powerful notion of maximum-margin separation between datapoints of different classes. Also, we gave insights of how model complexity is controlled by the hyperparameter W, and is independent of dimensions (in the high-dimensional setting).

We then presented another loss function: logistic loss or cross entropy loss or log loss defined by $l(x, y, w) \equiv \log\left(1 + e^{-yw^\top x}\right)$. The advantage is that this is a differentiable function, whereas the hinge-loss is not. Refer section 9.3 in Shalev-Shwartz and Ben-David [2014] for details.

[1] Infact a more comprehensive statement can be made: refer Feldman et al. [2009] for details.

Till now we focused our attention on explicitly modeling the Bayes optimal in a given Supervised Learning problem via the interesting idea of ERM over a specific inductive bias. The other alternative strategy is to directly model the underlying distribution in the given Supervised learning problem. If we succeed, i.e., if we estimate the joint likelihood p^* reliably using the training data, then we argued that the Bayes optimal can be deduced.

We showed that the Bayes optimal in case of regression problems with square-loss is given by the mean of the posterior likelihood[2]: $g^*(x) = E_{(X,Y)\sim p^*}[Y/X = x]$. We showed that the Bayes optimal in case of classification problems with 0-1 loss is given by the mode of the posterior likelihood: $g^*(x) \in \arg\max_{y\in\mathcal{Y}} p^*(y/x)$. In general, it was easy to see that the Bayes optimal was only a function of the posterior likelihood (and hence we don't even need to estimate the joint).

The above discussion leads to the following strategies for probabilistic modeling[3]:

Generative Modeling: Here the idea is to model the joint likelihood $p^*(x, y)$. From this the posterior $p^*(y/x)$ can be derived, using which the Bayes optimal can be found.

Discriminative Modeling: Here we directly model the posterior likelihood $p^*(y/x)$, using which the Bayes optimal is derived.

[2] We call $p^*(y/x)$ as the posterior likelihood (corresponding to $p^*(x, y)$).

[3] Because the objects being modeled are distributions, this is called as Probabilistic Modeling.

Lecture 7

(Parametric) Likelihood Estimation: MM & MLE

The key sub-problem to be solved in generative modeling is: given m iid samples $\mathcal{D} = x_1, \ldots, x_m$ from an unknown, yet fixed, likelihood p^*, estimate p^* as "accurately" as possible. We posed this problem as the following: $\min_{p \in D} \mathbb{L}(p, p^*)$, where D is the set of all (valid) likelihood functions and $\mathbb{L}$ is a 'loss' function that quantifies the disagreement between its argument likelihoods. We gave two examples of $\mathbb{L}$ functions: $\mathbb{L}_\phi(p, p^*) \equiv \|\mathbb{E}_{X \sim p}[\phi(X)] - \mathbb{E}_{X \sim p^*}[\phi(X)]\|$, where $\phi : \mathcal{X} \mapsto \mathbb{R}^d$ is any given function and $\mathbb{L}_{KL}(p, p^*) \equiv KL(p^* \parallel p) \equiv \mathbb{E}_{X \sim p^*}\left[\log\left(\frac{p^*(X)}{p(X)}\right)\right]$, is the KL divergence. In the KL divergence case, it is easy to see that the problem simplifies to: $\max_{p \in D} \mathbb{E}_{X \sim p^*}[\log(p(X))]$.

Analogous to ERM, we then approximated the expectation wrt. the underlying distribution p^* by the averages over training set. This approximation leads to the following problems: $\min_{p \in D} \left\|\mathbb{E}_{X \sim p}[\phi(X)] - \frac{1}{m}\sum_{i=1}^m \phi(x_i)\right\|$ and $\max_{p \in D} \frac{1}{m}\sum_{i=1}^m \log(p(x_i))$ respectively. As in case of ERM, such an (unrestricted) approximation fails miserably: in both cases we obtain the trivial solution $p(x_i) = \frac{1}{m}\ \forall\ i$. More importantly, these trivial solutions are the only solutions and they are completely useless for machine learning purposes!

Analogous to ERM with inductive bias, we then also restricted the search space of likelihood functions to obtain meaningful solutions. This leads to:

$$\min_{p \in \mathcal{P}} \left\|\mathbb{E}_{X \sim p}[\phi(X)] - \frac{1}{m}\sum_{i=1}^m \phi(x_i)\right\|, \tag{7.1}$$

and

$$\max_{p \in \mathcal{P}} \frac{1}{m} \sum_{i=1}^{m} \log\left(p(x_i)\right), \tag{7.2}$$

where $\mathcal{P} \subset D$ is an appropriate modeling bias, containing valid likelihood functions of a particular, loosely called as the probabilistic model. (7.1) is called as Method of Moments (MM), and (7.2) is called as Maximum Likelihood Estimation (MLE).

We then gave examples of models:

Bernoulli model: $\mathcal{M}_2$, the set of all likelihood functions corresponding to Bernoulli random variables. This model is parameterized by a single probability variable $\theta \in [0, 1]$. Refer section 2.3.1 in Murphy [2012].

Multinoulli model: $\mathcal{M}_n$, the set of all likelihood functions corresponding to Multinoulli random variables taking on n distinct values. This model is parameterized by $\theta \in \Delta_n$, where $\Delta_n \equiv \{z \in \mathbb{R}^n \mid z \geq 0, \sum_{i=1}^{n} z_i = 1\}$ (henceforth called as the n-dimensional simplex[1]. Needless to say, Multinoulli with $n = 2$ is same as Bernoulli. Refer section 2.4.1 in Murphy [2012].

(univariate) Gaussian Model: $\mathcal{G}_1$, the set of all (univariate) Gaussian likelihood functions. The common form of the likelihood function is $p_\theta(x) = \frac{e^{\frac{-1}{2\sigma^2}(x-\mu)^2}}{\sqrt{2\pi\sigma^2}}$. This is parameterized by $\theta = (\mu \in \mathbb{R}, \sigma^2 > 0)$.

(Multivariate) Gaussian Model: $\mathcal{G}_n$, the set of all n-dimensional Gaussian likelihood functions. The common form of the likelihood function is $p_\theta(x) = \frac{e^{\frac{-1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)}}{(2\pi)^{\frac{n}{2}}|\Sigma|^{\frac{1}{2}}}$. This is parameterized by $\theta = (\mu \in \mathbb{R}^n, \Sigma \succ 0 \in \mathbb{R}^{n \times n})$. Refer section 2.5.2 in Murphy [2012].

The details of MLE with $\mathcal{G}_1, \mathcal{G}_n$ are given in section 4.1.3 in Murphy [2012]. The MLE solution with $\mathcal{M}_2, \mathcal{M}_n$ follows from the weighted AM-GM inequality. In all these cases[2], we noted that the MM is the simplest and both MM, MLE give the same (usual) estimates for the parameters.

[1] Here, θ_i denotes the probability that the Multinoulli variable takes the i^{th} discrete value.

[2] This statement is true for any model in the so-called exponential family.

Lecture 8

Generative Models for Regression & Classification

We began with a special regression problem where $\mathcal{X} = \mathbb{R}^{n_1}, \mathcal{Y} = \mathbb{R}^{n_2}$. As discussed earlier, the key idea in generative modeling is to model the underlying input-output joint likelihood, $p^*(x, y)$.

Accordingly, we choose the $n_1 + n_2$ dimensional Gaussian as the model, i.e., $p(x, y) \sim \mathcal{N}(\mu, \Sigma)$. Let the parameters estimated (using MM or MLE) be $(\hat{\mu}, \hat{\Sigma})$. Let us define the following submatrices for the estimated parameters: $\hat{\mu} = \begin{bmatrix} \hat{\mu}_1 \\ \hat{\mu}_2 \end{bmatrix}$, and $\hat{\Sigma} = \begin{bmatrix} \hat{\Sigma}_{11} & \hat{\Sigma}_{21}^\top \\ \hat{\Sigma}_{21} & \hat{\Sigma}_{22} \end{bmatrix}$, where $\hat{\mu}_i \in \mathbb{R}_{n_i}, \hat{\Sigma}_{ii} \in \mathbb{R}^{n_i}$. We then wrote down a simplified expression for the posterior: $\hat{p}(y/x) \sim \mathcal{N}\left(\hat{\mu}_2 + \hat{\Sigma}_{21}\hat{\Sigma}_{11}^{-1}\left(x - \hat{\mu}_1\right), \hat{\Sigma}_{22} - \hat{\Sigma}_{21}\hat{\Sigma}_{11}^{-1}\hat{\Sigma}_{12}\right)$. Refer theorem 4.3.1 in Murphy [2012] for details of this derivation. Hence, the estimate for the Bayes optimal is the mean of this estimate posterior:

$$\hat{g}(x) = \hat{\mu}_2 + \hat{\Sigma}_{21}\hat{\Sigma}_{11}^{-1}\left(x - \hat{\mu}_1\right).$$

We commented that, apart from mean subtraction (normalization), the form of the function is linear, which is same as in case of linear regression. Henceforth, we will refer to the above as the generative linear regression model.

We then considered a classification problem in the special case $\mathcal{X} = \mathbb{R}^n$. Here it was clear that direct modeling of joint is not possible[1] with the limited set of basic models that we know of. The key idea was to indirectly model the joint by modeling the prior likelihood of the outputs, $p^*(y)$, and all the class-conditionals

[1] because, none of the named distributions we know of take on continuous and discrete values simultaneously!

$p^*(x/y) \; \forall \; y \in \mathcal{Y}$. Once these are estimated: $\hat{p}(y), \hat{p}(x/y)$, then using Bayes rule (for rvs), we have that the posterior likelihood is: $\hat{p}(y/x) = \frac{\hat{p}(x/y)\hat{p}(y)}{\sum_{y' \in \mathcal{Y}} \hat{p}(x/y')\hat{p}(y')}$. The Bayes optimal classifier is then obtained as mode of this estimated posterior. Classifiers thus obtained thus known as Bayes classifiers, and such a model is called Bayes classification model.

We then considered as an example, the Bayes classifier obtained when the class-conditionals are modeled with Gaussian and the prior using Multinoulli, henceforth refered to as Gaussian/Quadratic Discriminant Analysis (GDA/QDA). Refer section 4.2 in Murphy [2012] for details[2].

We ended by commenting that the advantages of Generative modeling (over ERM models) are:

1. Can now provide answers to questions like "what is the probability of rainfall being in $[90, 110]mm$?"
2. Can now compute the posterior (of outputs) given any partial observation of the inputs/outputs!

Whereas the disadvantage[3] is that the form of the final prediction function, $\hat{g}$ is difficult to guess/obtain, as it is not being directly modeled! Secondly, since modeling is done at a broader level (than necessarily required), the learning theoretic analysis is more involved.

[2]You may skip sections 4.2.6,4.2.8

[3]This issue will be gone in case of classification, once we consider models in exponential family.

Lecture 9

Discriminative models for Regression and Classification

In case of regression ($\mathcal{X} = \mathbb{R}^n, \mathcal{Y} = \mathbb{R}$), we motivated the following model (from experience in Generative modeling): $p_w(y/x) \sim \mathcal{N}(w^\top x, \sigma^2)$, where w, b are the parameters and σ^2 is a given hyper-parameter[1]. However, it seemed estimating the parameters is challenging (via MLE/MM) because for any x_i, only one sample for y is given in the training data!

From first principles, we then tried to derive an appropriate parameter estimation algorithm. Please refer page 2 in `https://www.iith.ac.in/~saketha/teaching/cs5560Scribe.pdf` for details. This leads to the following method for parameter estimation, called as Maximum Conditional Likelihood Estimation (MCLE):

$$\max_{w \in \mathcal{W}} \frac{1}{m} \sum_{i=1}^{m} \log \left(p_w(y_i/x_i) \right), \tag{9.1}$$

where $\mathcal{W}$ is the set of permissible values of the parameter.

Please refer section 7.3 in Murphy [2012] for MCLE estimation for the above discriminative regression model. Interestingly, the final prediction function $\hat{g}$ turns out to be exactly same as that in case of linear regression. Hence this model is also called as Linear Regression. The only difference between this discriminative model and the ERM one is that this additionally provides posterior likelihood for the outputs.

We then moved on to the case of classification. Again, motivated by the Bayes classification model, we considered the discriminative model[2]: $p_{w,b}(y/x) \sim$

[1] See also section 7.2 in Murphy [2012]

[2] Refer also section 8.2 in Murphy [2012].

$Mul(\theta_1(w,b),\ldots,\theta_c(w,b))$, where $\theta_i(w,b) = \frac{e^{w_i^\top \phi(x)}}{\sum_{j=1}^{c} e^{w_j^\top \phi(x)}}$. Refer section 8.3.1, 8.3.7 in Murphy [2012] for details of MCLE in this case. Interestingly, we found that in the special case of binary classification, the MCLE problem is exactly same as the ERM with logistic regression (without regularization). So, this model is also called as Logistic Regression. One has to resort to numerical solvers like gradient descent etc. to solve this optimization problem. Interested students may refer section 8.3.2 in Murphy [2012] for details of gradient descent in this case.

Motivated by this discriminative logistic regression model, we presented the following non-probabilistic model for solving a (multi-class) classification problem: the key idea is to model

$$\log(p(y/x))) \propto w_y^\top \phi(x) \tag{9.2}$$

Modeling scores proportional to relevant log-likelihood functions is indeed a fundamental idea in non-probabilistic modeling. The final prediction function is then given by: $\hat{g}(x) = \arg\max_{y\in\mathcal{Y}} w_y^\top \phi(x)$. The 0-1 loss in this case is given by: $l_{01}(y,w,x) = 1_{y\neq \arg\max_{z\in\mathcal{Y}} w_z^\top \phi(x)} = 1_{\max_{z\neq y\in\mathcal{Y}} w_z^\top \phi(x) > w_y^\top \phi(x)}$. The hinge-loss is given by

$$l(y,w,x) = \max\left(0, 1 - \left(w_y^\top \phi(x) - \max_{z\neq y\in\mathcal{Y}} w_z^\top \phi(x)\right)\right).$$

Regularized ERM with this hinge-loss is called as the Multi-class SVM model[3].

Finally we concluded with noting trade-offs with Generative vs Discriminative models. This is summarized nicely in section 8.6 in Murphy [2012].

[3] If interested please refer section 17.2 in Shalev-Shwartz and Ben-David [2014] for more details.

Lecture 10

Non-linear Models and Exponential Family

We generalized the $\mathcal{L}_W$ model to $\mathcal{F}_W \equiv \left\{ f \mid \exists w \in \mathbb{R}^d, \|w\| \leq W \ \ni \ f(x) = w^\top \phi(x) \ \forall \ x \in \mathcal{X} \right\}$, where $\phi : \mathcal{X} \mapsto \mathbb{R}^d$, is a given feature map. We call this the Non-linear Model or the generalized linear model. Note that the model is defined once ϕ, W are fixed. So we infact defined a huge family of models! The advantages of such models is obvious: for example, can be used if the Bayes optimal is known to be a non-linear function etc. Also, such models work with any arbitrary input space rather than $\mathbb{R}^n$ alone. Infact, designing models will now essentially be same as designing the feature map ϕ using domain knowledge in the relevant application. Hyperparameter, W, is typically chosen using model selection techniques from the subsequent lecture.

The general (Tikhonov) form for the ERM problem with such models turns out to be:

$$\min_{w \in \mathbb{R}^d} \frac{1}{2}\|w\|^2 + C \sum_{i=1}^{m} l\left(y_i, w^\top \phi(x_i)\right). \tag{10.1}$$

This together with square loss, and ϵ-insentive loss give the "non-linear" generalizations of the Ridge-regression, and SVR models respectively. This together with the hinge-loss, and logistic loss give the "non-linear" generalizations of the SVM, and logistic regression models.

We then generalized the probabilistic models in an analogous way. Given a map $\phi : \mathcal{X} \mapsto \mathbb{R}^d$, we consider the set of likelihoods of the form:

$$p_w(x) = \frac{e^{w^\top \phi(x)}}{Z(w)}, \tag{10.2}$$

where w is the parameter, $Z(w)$ is the normalization constant. Likelihoods parameterized by w, for a fixed ϕ from the model. We call ϕ as sufficient statistics and Z as the partition function. We call the family of such models (one for each ϕ) as the exponential family of models. Here too, designing the model is same as designing the sufficient statistics[1], ϕ. The form of the likelihood in (10.2) is sometimes[2] also referred to as the Gibbs distribution or Boltzmann distribution corresponding to the energy function $w^\top \phi(\cdot)$.

In case of generative modeling, one would use an exponential family model with an appropriate $\phi(x, y)$. The details of MLE/MM with such models is presented in `https://1drv.ms/b/s!Au6Zdrbq2x4ph7RpGBT7D9PGSAkozg?e=gqv77x`.

In case of discriminative modeling, one would use an exponential family model with an appropriate sufficient statistics $\phi(y) : \mathcal{Y} \mapsto \mathbb{R}^{d_2}$. However, the parameters will be some functions of the observed (input) variable x. We represent the i^{th} parameter (corresponding to $\phi_i(x)$) by $w_i^\top \psi(x)$, where $\psi : \mathcal{X} \mapsto \mathbb{R}^{d_1}$ is a given feature map. This leads to the following form for the likelihood:

$$p_w(y/x) = \frac{e^{\psi(x)^\top W \phi(y)}}{Z\left(W, \psi(x)\right)},$$

where W is the parameter matrix with i^{th} column as w_i. The details of MLE/MM with such models is presented in `https://1drv.ms/b/s!Au6Zdrbq2x4ph7RqM1dNyd1wu4qu3A?e=3MPA0z`.

To summarize the three main modeling frameworks: Using domain knowledge, in generative models, the joint sufficient statistics $\phi(x, y)$ are designed[3], in discriminative models, the sufficient statistics over outputs[4] $\phi(y)$ and the feature map over inputs $\psi(x)$ are designed, in non-probabilistic models, the feature map over inputs[5] are typically desgined

We finished the lecture by noting that in some cases the ERM problem with the non-linear models (10.1) can be solved efficiently even in high-dimensional cases. We noted that in case one wants to deal with a feature map that induces all possible r degree monomials over the input factors in $\mathbb{R}^n$, then $d = O(n^r)$. In such cases, or essentially cases where d is high, solving the ERM problem may be computationally challenging. We then made the observaion that the optimal

[1] Typically, this designing is done using the language of undirected grahical models. Interested students may refer section 19 in Murphy [2012].

[2] This is a terminology from Statistical Physics.

[3] MRFs (chapter 19 in Murphy [2012]) are typically used here.

[4] CRFs (section 19.6 in Murphy [2012]) are typically used here.

[5] Infact, joint feature maps over inputs and outputs in the most general design. For e.g., refer `structSVM` in section 19.7 in Murphy [2012] or for eg., `http://www.jmlr.org/papers/volume17/11-315/11-315.pdf` operator-valued kernel methods.

solution of the ERM (10.1) will always be a linear combination of the feature maps of the training inputs. This is called as the representer theorem:

Theorem 10.0.1. *Any optimal solution, $\hat{w}$, of (10.1) will be of the form $\hat{w} = \sum_{i=1}^{m} \alpha_i \phi(x_i)$. Hence (10.1) is equivalent to:*

$$\min_{\alpha \in \mathbb{R}^m} \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j k\left(x_i, x_j\right) + C \sum_{i=1}^{m} l\left(y_i, \sum_{j=1}^{m} \alpha_j k\left(x_i, x_j\right)\right), \tag{10.3}$$

where $k\left(x_i, x_j\right) \equiv \phi(x_i)^\top \phi(x_j)$. Also, $\hat{w}^\top \phi(x) = \sum_{i=1}^{m} \alpha_i k\left(x_i, x\right) \quad x \in \mathcal{X}$.

Refer section 4.2 in Scholkopf and Smola [2001] or theorem 5.4 in Mohri et al. [2012] for details of the proof.

From the theorem it is clear that the ERM is independent of the dimensionality d, as long as the computation of the dot product, i.e., evaluation of the function k, is (computationally efficient). Interestingly, we noted that with $k(x, z) \equiv \left(x^\top z\right)^r$, one induces a feature map with all possible r degree monomials! And, with $k(x, z) \equiv \left(1 + x^\top z\right)^r$, one induces a feature map with all possible monomials upto degree r degree. Since $\hat{w}^\top \phi(x) = \sum_{i=1}^{m} \alpha_i k\left(x_i, x\right)$, the ERM is indeed independent of d (for computational purposes) as long as the Bayes optimal is a polynomial. In the subsequent lecture we will introduce a generic definition for k that will help us induce other forms for the Bayes optimal as well.

Lecture 11

Kernels and Model Selection

Encouraged by the implications of the representer theorem, we asked the converse question: what are the properties that need to be satisfied by a function $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$, such that $k(x, z)$ represents an inner-product in some space? Without giving any justification/proofs[1], we defined such functions as kernels: a function $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is said to be kernel over $\mathcal{X}$ iff for every $m \in \mathbb{N}$ and for every $z_1, \ldots, z_m \in \mathcal{X}$, the corresponding gram matrix, G, is positive semi-definite. Gram matrix is defined as that with i, j entry as $k(z_i, z_j)$. We then wrote many theorems (without proof) that will help one verify that a given function is a kernel or not.

Theorem 11.0.1. *If $\exists\ \phi : \mathcal{X} \mapsto \mathbb{R}^d$ (for some $d \in \mathbb{N}$), such that $k(x, z) = \phi(x)^\top \phi(z)$, $\forall\ x, z \in \mathcal{X}$, then k is a kernel over $\mathcal{X}$.*

Theorem 11.0.2. *If $k_1, \ldots, k_n$ are kernels over $\mathcal{X}$ and $\alpha_i \geq 0\ \forall\ i = 1, \ldots, n$, then $k \equiv \sum_{i=1}^n \alpha_i k_i$ is a kernel over $\mathcal{X}$.*

Theorem 11.0.3. *If $k_1, \ldots, k_n$ are kernels over $\mathcal{X}$, then $k \equiv \Pi_{i=1}^n k_i$ is a kernel over $\mathcal{X}$.*

Theorem 11.0.4. *If $k_1, \ldots, k_n, \ldots$ is an infinite sequence of kernels over $\mathcal{X}$, then $\lim_{n\to\infty} k_n$ exists and that limiting[2] function will be a kernel over $\mathcal{X}$.*

Theorem 11.0.5. *If k is a kernel over $\mathcal{X}$, then the normalized[3] function defined by $\bar{k}(x, z) \equiv \frac{k(x,z)}{\sqrt{k(x,x)}\sqrt{k(z,z)}}\ \forall\ x, z \in \mathcal{X}$ will be a kernel over $\mathcal{X}$. We will call $\bar{k}$ as the normalized[4] version of k.*

[1] Interested students may refer section 2.2.2 in Scholkopf and Smola [2001] for proofs.
[2] Refer theorem 5.3 in Mohri et al. [2012] for a proof of theorems 11.0.1-11.0.3.
[3] Refer lemma 5.2 in Mohri et al. [2012] for a proof.
[4] Or k as the un-normalized version of $\bar{k}$.

Using the above, we can show that the following are valid kernels[5] over $\mathbb{R}^n$:

Linear Kernel: $k_{a,\Sigma}(x,z) \equiv x^\top \Sigma z + a$, where $a \geq 0, \Sigma \succeq 0 (\neq 0)$ are the parameters[6] of the kernel. The form of prediction function with this kernel will be linear/affine: $w^\top \phi(x) = \sum_{i=1}^m \alpha_i \left(x_i^\top \Sigma x + a \right)$.

Polynomial Kernel: $k_{a,\Sigma,r}(x,z) \equiv \left(x^\top \Sigma z + a \right)^r$, where $r \in \mathbb{N} (\neq 1), a \geq 0, \Sigma \succeq 0 (\neq 0)$ are the parameters of the kernel. The form of prediction function with this kernel will be (upto) r^{th} degree polynomial: $w^\top \phi(x) = \sum_{i=1}^m \alpha_i \left(x_i^\top \Sigma x + a \right)^r$.

Gaussian/RBF kernel: $k_\Sigma(x,z) \equiv e^{-\frac{1}{2}(x-z)^\top \Sigma (x-z)}$, where $\Sigma \succeq 0 (\neq 0)$ are the parameters of the kernel. Typically one restricts $\Sigma = \frac{1}{\sigma^2} I$. The form of prediction function with this kernel will be linear combinations of Gaussian functions.

With each of these kernels, we can now kernelize ERM models using theorem 10.0.1, leading to kernelized linear/Ridge/SVM-regression, and kernelized SVM/logistic regression. Note that the parameters of the kernel employed will now be the hyper-parameters of the respective models. Refer chapter 16 in Shalev-Shwartz and Ben-David [2014] for details. Infact, such a kernelization trick can be employed with any algorithm/model that involves only information about inner-products and consequent quantities related to the data.

At this stage, we have access to many modeling frameworks:

ERM based non-linear models: Here, the main artifacts in model design are the feature map $\phi : \mathcal{X} \mapsto \mathbb{R}^d$, and the loss function, both of which need to be designed carefully using application domain expertise: since ϕ explicitly determines the form of the Bayes optimal, it must be chosen appropriately. The hyperparameters are: C, and the parameters of the loss function (if any).

Generative models from Exponential family: Here, the sufficient statistics $\phi : \mathcal{X} \times \mathcal{Y} \mapsto \mathbb{R}^d$ are to be designed[7] carefully using domain expertise.

Discriminative models from Exponential family: Here, the sufficient statistics $\phi : \mathcal{Y} \mapsto \mathbb{R}^{d_2}$ and the feature map $\psi : \mathcal{X} \mapsto \mathbb{R}^{d_1}$ are to be carefully designed[8].

[5] Refer section 2.3 in Scholkopf and Smola [2001] for more examples including those over non-Euclidean spaces.

[6] Parameters of the kernel will naturally be the hyperparameters in corresponding kernelized models.

[7] Markov random fields or undirected graphical models are popularly used to this design.

[8] Conditional Random Fields are popular here.

ERM based kernel methods: Here, the kernel function over input space[9] needs to be carefully designed using domain expertise: the kernel must intuitively represent notion of similarity between inputs, and since the kernel function's form determines that of the final prediction function, it must be chosen to include the Bayes optimal. The hyperparameters are C, the parameters of the loss (if any) and parameters of the kernel (if any). Needless to say, a kernel can be designed by designing feature map $\phi : \mathcal{X} \mapsto \mathbb{R}^d$. But that is not necessary!

As we can see, even after careful design, the values of hyperparameters remain largely unknown. Also, one may not have enough domain knowledge to make a choice between the models in these various frameworks. In such a case, one has to deal with the problem of hyper-parameter estimation or that of selecting the "best" of these seemingly equivalent[10] models. This problem is known as the problem as Model Selection. Let the models (hyperparameters) be $\mathcal{M}_1(\vartheta_1), \ldots, \mathcal{M}_n(\vartheta_n)$.

Since training data is reserved for parameter estimation, and domain expertise is used-up in model design, one needs access to extra independent information, called the Validation/Development (Dev) data for performing hyperparameter estimation or Model selection. We assume that the samples in the Validation and Training sets are all iid from the same underlying, unknown, $p^*(x, y)$. Section 11.2 in Shalev-Shwartz and Ben-David [2014] is an excellent reference for model selection.

With this set-up, hyper-parameter estimation or model selection can simply be done using ERM but now using Validation data. This is called as Validation procedure:

1. Using Training data, we estimate (using ERM/MM/MLE/MCLE) the parameters in (with) each model (hyperparameter): $\hat{\theta}_1, \ldots, \hat{\theta}_n$.
2. Using Validation/Dev data, we estimate (using ERM) the hyperparameter i.e., pick the model/hyperparameter whose $\hat{\theta}$ gives least average Validation set error. Let the index of this model (hyperparameter) be $\hat{i}$.
3. The final prediction function is that obtained by performing parameter estimation in the $\hat{i}^{th}$ model using ERM/MM/MLE/MCLE over the entire training and validation data together. Let this parameter be .

One shortcoming with the above procedure is that the hyperparameter estimation (model selection) is done using only m_v no. datapoints, though the final

[9] These can be generalized to methods that involve kernels over output space too: Tsochantaridis et al. [2004] (`StructSVM`).

[10] Equivalent in terms of satisfying the domain knowledge based constraints.

parameter estimation is done using $m_t + m_v$ no. datapoints. Here, m_t, m_v denote the sizes of the training, validation sets respectively. Using clever re-sampling one can handle this asymmetry and make it appear as if $m_t + m_v$ datapoints are used for both parameter and hyperparameter estimation. An example of such a clever technique is k-fold Cross-Validation (CV). Please refer section 7.10 in Hastie et al. [2001] for details. When number of folds is same as $m_t + m_v$, this procedure is called as Leave One Out (LOO) CV. In general, given enough samples, LOO error is a better estimate for the true risk than k-fold CV, which is in turn a better estimate than the validation set error[11].

We finally commented that questions like which set of models are to be considered (hyperhyperparameter estimation :) can be again answered if additional data (hypervalidation data :) is given and so on... However, usually one stops at the level of hyperparameter estimation. Hence it is extremely important to decide on the set of models to be considered purely based on domain expertise and other learning considerations, and never after number crunching over the training/validation datasets!

We end by clarifying what the so-called test/evaluation data is. This is again mutually independent data from the underlying $p^*(x, y)$. However, this is **NEVER** available to the machine learning algorithm or the ML designer/researcher/developer. This is data used to approximate the true risk in employing the final prediction function returned by the ML algorithm. Purely for the purposes of academia[12], test data is also published with the understanding that it will be used at no stage in the ML pipeline. In real-world deployment, test set is never published. Needless to say, lesser the error on test data, better the classifier/regressor. Like-how ML is guaranteed to succeed only with huge amounts of training and validation data, evaluation is guaranteed to succeed only if the test data size is also huge.

[11] Bagging, covered later on, also uses similar ideas.

[12] In other words, in academia, the given data is split in three parts training, validation, test such that the joint distributions are maintained. Then test data is never used except for the final evaluation.

Lecture 12

Non-Parametric Methods: Nearest Neighbour methods

We started looking at a completely different kind of modeling where the very notions of inductive bias or parameters are very non-standard. We began with the example of Nearest Neighbor (NN) algorithm. Please refer section 13.3 in Hastie et al. [2001], which gives a nice overview of this method. Also, chapter 19 in our textbook Shalev-Shwartz and Ben-David [2014] presents simple yet insightful analysis of such algorithms for the case of binary classification.

Here the model is extremely simple: the idea is to remember/store the entire training data and when a (new) input is given, search for the nearest input in the training data and assign the label of the (new) input as that of this nearest input.

We began by analyzing this model/classifier formally. The formal analysis is due to Cover and Hart [1967][1]. The key result from this work is, under mild conditions and as $m \to \infty$ (m is number of training examples), we have

$$0 \leq R^* \leq R^{NN} \leq R^* \left(2 - \frac{c}{c-1} R^*\right),$$

where R^{NN} denotes the expected misclassification error of the NN classifier, in the limit and c is the number of classes. We also commented on two extreme cases: i) if $R^* = 0$, then the bounds are tight and $R^{NN} = 0$. Algorithms that achieve Bayes error are said to be Bayes consistent. Moreover, if $R^* = 0.5$ (supervisor is clueless), then $R^{NN} = 0.5$ (so will be the learner).

We then thought about an improvement for reducing the chance of picking a low probability label from the neighbour. The obvious idea was to look for some

[1] Available at `https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=1053964`

k nearest neighbours instead of one and take the majority vote, henceforth called as the k-NN classification algorithm. And because for large k, we expect majority vote to be the same as the more probable class, the error might reduce to R^*.

We intuitively argued that $m \to \infty, k \to \infty, \frac{k}{m} \to 0$ will be the conditions under which error will reduce to R^*. This intuitive result is formally stated in the following theorem (proof skipped) due to Devroye and Gyorfi [1985][2]:

Theorem 12.0.1. *If $\mathcal{X} \subset \mathbb{R}^n, \mathcal{Y} = \{-1, 1\}$ and under the conditions $k \to \infty, \frac{k}{m} \to 0$, we have with atleast $1 - \delta$ probability,*

$$R_m^{kNN} - R^* \leq \sqrt{\frac{72\gamma^2 \log \frac{2}{\delta}}{m}},$$

where R_m^{kNN} denotes the expected probability of misclassification with k-NN classifier trained with m examples and $\gamma \leq \left(1 + \frac{2}{\sqrt{2-\sqrt{3}}}\right)^n - 1$.

Though this theorem shows that $k-NN$ is Bayes consistent, one must not be overwhelmed because it is merely an asymptotic result ($m \to \infty, k \to \infty, \frac{k}{m} \to 0$). Bounds that are more interesting are those with finite m, k. We were able to say something about the finite k binary classification case, which is formalized in the following bound[3]:

$$0 \leq R^* \leq \ldots R^{(2k+1)NN} \leq R^{(2k-1)NN} \leq \ldots \leq R^{3NN} \leq R^{NN} \leq 2R^*(1 - R^*),$$

where R^{kNN} denotes the limiting value of the expected misclassification error with the k-NN classifier, as $m \to \infty$. Refer pages 2-5 in `https://1drv.ms/b/s!Au6Zdrbq2x4p9lpB0HH56uJPWbFK?e=qhwBhv` for a sketch of proof. Section 19.2 in our textbook Shalev-Shwartz and Ben-David [2014] gives an alternative simple yet insightful analysis but is limited to $1-NN$, however deals with finite m (e.g., theorem 19.3). Most insightful is theorem 19.5 that deals with finite m, k, however we skip proofs of both these theorems. An important insight from theorem 19.5 is that the $k-NN$ suffers from the curse of dimensionality (similar to unbounded linear models)!

If one needs to solve a regression problem, then the average output of the k nearest neighbours is used as the prediction function. This is known as k-NN regression. Motivated with the ideology of k-NN, we present algorithms for estimating likelihoods, which will help us build probabilistic models (in subsequent lecture).

[2]Please refer chapter 11, theorem 11.1, in ? for a detailed proof.
[3]Please refer chapter 5, theorem 5.4, in ? for an insightful proof

We argued that kernelized SVMs (which are parametric), can also be understood as non-parametric methods. Here are some trade-marks for identifying non-parametric methods:

1. Assumptions regarding the form of prediction function are either absent or not as strong as in case of parametric methods.
2. Parameters for the model cannot be identified or if identified will grow with the number of samples.
3. After training, for the purposes of inference, one needs to store some or all of the training data in some form or the other.
4. Under mild conditions, asymptotically, Bayes consistency is achieved[4].

We concluded by summarizing the pros and cons of nearest neighbour methods:

Pros:
1. Even though asymptotically, Bayes consistency is guaranteed. Such a guarantee is difficult to provide in parametric models[5].
2. Simple and intuitive algorithm to understand.
3. Can employ any distance function that is natural in the ML application.

Cons:
1. These methods are plagued with the curse of dimensionality (theorem 19.5 in Shalev-Shwartz and Ben-David [2014])!
2. For high dimensional problems and those with unyielding complicated distance functions, the computational cost is substantially high[6].
3. Coding can be involved if it has to be done efficiently or if non-standard distance functions are employed.
4. Intuitively difficult to generalize such methods to problems other than classification and regression. For e.g., those in structured prediction.

[4]SVMs with Gaussian kernel again can be showed to achieve Bayes consistency, asymptotically. For e.g., refer `http://members.cbio.mines-paristech.fr/~jvert/svn/bibli/local/Steinwart2005Consistency.pdf`.

[5]Exception is (Gaussian) kernelized SVMs etc., where such a guarantee can be given (again asymptotically). However, the beauty in SVMs is that they is no curse of dimensionality.

[6]Nearest neighbour finding is a standard problem studied in CS with huge amount of literature.

Lecture 13

Non-parametric likelihood estimation

We re-looked at the problem of likelihood estimation: given m iid samples from an unknown, yet fixed, likelihood p^*, estimate this likelihood function. Now we want to perform this estimation in a non-parametric way i.e., without assuming strong assumptions on the form of the likelihood function etc., like in k-NN.

We simply follow section 14.7.2 in Murphy [2012], which leads to Kernel Density Estimation (KDE). Smoothing kernels are defined in section 14.7.1 in Murphy [2012]. From this non-parametric estimation, the following methods are immediate:

Discriminative Regression: Estimate for $p^*(y/x)$ is the KDE with outputs of the k nearest neighbours of x.

Discriminative Classification: Estimate for $p^*(y/x)$ is the fraction of the k nearest neighbours of x, which have output as y. This is described in section 14.7.3 in Murphy [2012].

Generative Regression: This is described in section 14.7.4 in Murphy [2012].

Generative Classification: Here again the idea is to build a bayes classifier, but now using non-parametric models[1] for $p^*(x/y)$. In particular, we use KDE for esitmating $p^*(x/y)$ for each class y: $\hat{p}(x/y) = \frac{1}{m_y} \sum_{i:y_i=y} \kappa_h(x - x_i)$, where m_y is no. training samples with label as y. Let $\hat{\Pi}_y$ be the estimate for $p^*(y)$.

[1] It is easy to see that $p(y)$ estimation remains the same whether parametric or non-parametric! This is because we use multinoulli, which is the the most general discrete distribution.

The by Bayes rule, $p(y/x) \propto \frac{\hat{\Pi}_y}{m_y} \sum_{i:y_i=y} \kappa_h(x - x_i)$ and the corresponding Bayes classifier is simply the mode (as function of the input).

Lecture 14

Unsupervised Learning: 1-class SVM, Mixture Models

We began considering learning tasks that are very different than the Supervised learning tasks dealt with till now. We introduced unsupervised learning through example problems:

1. We defined that likelihood estimation is an example of unsupervised learning! This is because: if it were a supervised learning problem, then one would have been given for each training sample, the corresponding likelihood. For this unsupervised learning problem we already know estimation methodologies: MM,MLE,MCLE and KDE.

2. The problem of identifying high-likelihood (density) regions using iid samples from it:

   (a) Again, this is naturally unsupervised because the very fact that a sample is sampled means is most likely belongs to high density regions (otherwise it has low likelihood of being sampled :)

   (b) The applications of novelty/intrusion/anomaly detection can be solved by solving this unsupervised problem. Here, novel/anomaly points are simply those that are less likely.

   (c) The applications of clustering can be solved by solving this unsupervised problem. We define clusters as contiguous regions of high-likelihood. Section 25.1 in Murphy [2012] gives an alternative, yet intuitively equivalent[1], definition for clusters, which is that of set of close by points.

[1] I personally prefer the high-likelihood view of clustering.

We began with parametric non-probabilistic models for high-likelihood region estimation problem. Similar to multiclass SVM (9.2), the idea was to model a quantity proportional to the log-likelihood: $\log\left(p^*(x)\right) \propto w^\top \phi(x)$. And, define the final prediction function as $\hat{g}(x) \equiv \begin{cases} \text{high} & \text{if } \hat{w}^\top \phi(x) > 0 \\ \text{low} & \text{if } \hat{w}^\top \phi(x) \leq 0 \end{cases}$. The natural loss was the hinge-loss $l(\text{high}, w, x) \equiv \max\left(0, 1 - w^\top \phi(x)\right)$. This leads to the following ERM (henceforth referred to as one-class SVM[2]):

$$\min_{w \in \mathbb{R}^d} \frac{1}{2}\|w\|^2 + C \sum_{i=1}^{m} \max(0, 1 - w^\top x_i)$$

In novelty detection applications, one can simply declare "low" likelihood points as "novel". In clustering applications, one needs to perform post-processing[3] for cluster assignments:

1. Let $\mathcal{I}$ be the index set of those points labeled "high" by the one-class SVM.
2. We initialize the adjacency matrix, A, representing cluster information with $A_{ij} = 0 \; \forall \; (i, j) \in \mathcal{I} \times \mathcal{I}$.
3. For each pair in $(i, j) \in \mathcal{I} \times \mathcal{I}$, we verify if the points in the line segment between the pair are also labeled "high". If so, then $A_{ij} = 1$.
4. Clusters are defined as the connected components in A. Note that such a procedure would indeed retrieve contiguous regions of high density (as per the model).

The key advantages of such a clustering, henceforth referred to as Support Vector Clustering (SVC), are that the number of clusters need not be known aprior and no strong assmptions on the shapes of clusters need to be made. The limitations are: i) tuning the hyperparameters[4] like C and kernel parameters is difficult ii) the algorithm for cluster assignment does not computationally scale well to large datasets.

We then moved on to parametric probabilistic models. The obvious strategy was to estimate likelihood and then compute high likelihood regions. However,

[2] Interested readers may refer (3.4) in `http://users.cecs.anu.edu.au/~williams/papers/P132.pdf` for a more generalized formulation, which is equivalent to (3.13) in the paper for Gaussian kernels.

[3] Refer `http://www.jmlr.org/papers/volume2/horn01a/horn01a.pdf` for details in an equivalent formulation.

[4] One can still do something like CV but with disagreement over various folds wrt. clusters as the CV error.

we motivated mixture models for clustering applications rather than using exponential family models.

Given c likelihood models $\mathcal{M}_1, \ldots, \mathcal{M}_c$ (over $\mathcal{X}$), the corresponding mixture model is defined as

$$\mathcal{M} \equiv \left\{ p \mid \exists p_i \in \mathcal{M}_i \; \forall \; i = 1, \ldots, c, \exists \alpha \in \Delta_c \; \ni \; p(x) = \sum_{i=1}^{c} \alpha_i p_i(x) \; \forall \; x \in \mathcal{X} \right\}.$$

For a given $p \in \mathcal{M}$, the corresponding α_i are called as mixing coefficients and the corresponding $p_i \in \mathcal{M}_i$ are called as the component likelihoods (or simply components). If all component models are Gaussian, then the mixture model is called as the Gaussian Mixture Model (GMM). The key advantages of mixture modeling are:

1. Mixture models need not belong to exponential family, even if all component models belong to the exponential family. Thus it provides a new family of probabilistic models, which can now be used in generative/discrminative models for supervised learning!

2. During identifying high density regions is now easy! They are only c well-defined likelihoods!

The limitations are c, the no. components, need to be estimated (separately) and is challenging. The form of the clusters is strongly determined by the form of the component sufficient statistics! Refer section 11.2 in Murphy [2012] for details on mixture model. Details of the MLE problem and its solving by Expectation Maximization (EM) algorithm are summarized in sections 11.3,11.4-11.4.2.4. The EM derivation from the lecture is here: `https://1drv.ms/b/s!Au6Zdrbq2x4ph7c8CCv2C8hjef-sig?e=NDT5k9`.

Lecture 15

Non-parametric Clustering

We began by commenting that the parameter update equations in the EM algorithm are intuitive and simply the weighted-average versions of the usual formulae:

$$\begin{aligned}\mathbb{E}_{w_y^{(k)}}\left[\phi(X)\right] &= \frac{\sum_{i=1}^m p_{w^{(k-1)}}(y/x_i)\phi(x_i)}{\sum_{i=1}^m p_{w^{(k-1)}}(y/x_i)} \\ \alpha_y^{(k)} &= \frac{\sum_{i=1}^m p_{w^{(k-1)}}(y/x_i)}{m}\end{aligned}$$

Here, $\left(w^{(k)}, \alpha^{(k)}\right)$ denote the parameter values in k^{th} iteration. The above is called the M-step. The posterior can be computed using: $p_{w^{(k)}}(y/x_i) \propto \alpha_y^{(k)} e^{\left(\left(w_y^{(k)}\right)^\top \phi(x_i)\right)}$. This is called as the E-step.

One way to perform non-parametric clustering is by kernelizing the SVC formulation. An alternative is the so-called k-means clustering, which is a special case of the above EM based mixture modeling:

1. Consider a GMM with k components.
2. Assume all the components that equal and spherical covariance, I.
3. Assume all the mixing coefficients are equal to $\frac{1}{k}$. In other words, the only parameters are the means of each component $\mu_1, \ldots, \mu_c$.
4. Instead of the standard EM updates, we keep the M-step the same, but change the E-step to (hard thresholding):

$$p_{w^{(k)}}(y/x_i) = \begin{cases} 1 & \text{if } y = \arg\max_{z \in \mathcal{Y}} \alpha_z^{(k)} e^{\left(\left(w_z^{(k)}\right)^\top \phi(x)\right)} \\ 0 & \text{otherwise,} \end{cases}$$

which by above modeling assumptions further simplifies to:

$$p_{w^{(k)}}(y/x_i) = \begin{cases} 1 & \text{if } y = \arg\min_{z \in \mathcal{Y}} \|x_i - \mu_z^{(k)}\|^2 \\ 0 & \text{otherwise,} \end{cases}$$

We noted that the lower bound (proxy objective) obtained by the Jensen's inequality in this case is given by:

$$\min_{\mu_1,\ldots,\mu_c} \sum_{j=1}^{c} \sum_{i \in S_j} \|x_i - \mu_j\|^2 \tag{15.1}$$

where, $S_j \equiv \{i \in 1,\ldots,m \mid j = \arg\min_{z \in \mathcal{Y}} \|x_i - \mu_j\|^2\}$. In other words, the proxy clustering objective is minimizing the within-cluster variance! Infact, many consider this proxy (15.1) as the definition of clustering[1], where the Euclidean distance can be replaced by any valid distance function. When the distance is induced by a kernel: $d(x,y) \equiv \sqrt{k(x,x) + k(y,y) - 2k(x,y)}$, then it is called as kernelized k-means clustering.

Unfortunately, (15.1) is a computationally intractable (Aloise et al. [2009]) problem, even with the Euclidean distance. The k-means algorithm can be understood as a greedy algorithm for approximately solving it (not guaranteed to find the optimum).

We finished the lecture by briefly discussing Hierarchical clustering (see section 25.5 in Murphy [2012]) and graph-based methods (see section 22.3.1 in Shalev-Shwartz and Ben-David [2014]).

[1] However, this objective is a relaxed (lower bound) version of the (true) high-density objective.

Lecture 16

Representation Learning: PCA

Representation learning is yet another unsupervised learning problem, where (informally) the goal is to learn the feature-map/sufficient-statistics/kernel using (additional) data. One generic optimization problem that captures the goal in representation learning (in the unsupervised setting) is:

$$\min_{f \in \mathcal{F}, g \in \mathcal{G}} \mathbb{E}[l(X, f \circ g(X))], \tag{16.1}$$

where $\mathcal{G}, \mathcal{F}$ are sets of representation, reconstruction maps, and l is a loss function. Note the similarity/differences between the ideal objectives of supervised learning (3.1) and (unsupervised) representation learning (16.1).

We detail the special case of dimensionalty reduction: where one needs to refine the pre-designed feature map $\phi : \mathcal{X} \mapsto \mathbb{R}^d$ such that the dimensionality is reduced from d to $r << d$. Motivations for such a reduction are listed in the beginning of chapter 23 in Shalev-Shwartz and Ben-David [2014]. In terms of (16.1), $\mathcal{G}$ is a set of functions from $\mathbb{R}^d \mapsto \mathbb{R}^r$, and $\mathcal{F}$ from $\mathbb{R}^r \mapsto \mathbb{R}^d$, and l is say, square-loss. The corresponding ERM, with inductive bias chosen as linear, is given by (23.1) in Shalev-Shwartz and Ben-David [2014].

Using lemma 23.1, we then re-wrote (23.1) as (23.4), which is a well-studied problem in linear algebra. It so happens that this is a terribly non-convex problem, yet can be efficiently solved using Eigen Value Decomposition (EVD) in $O(d^3)$ computations. The details of EVD based solution is presented in theorem 23.2. This is known as Principal Component Analysis (PCA).

Infact, the PCA can be kernelized, the details of which are presented in sections 23.1.1, 23.1.2. The computational effort for kernelized PCA is $O(m^3)$ as it involves EVD of the gram matrix induced by the kernel.

Motivated by the series of compositions of functions that exist in kernelized

PCA, we then presented the Autoassociative Neural Network model (autoencoder networks) detailed in section 12.4.2 in Bishop [2006]. Based on this discussion we defined a new (non-probabilistic) model: (feedforward non-recurrent) neural network or multilayer perceptron, which is functions of the form:

$$f_W(x) \equiv w^\top \left(\sigma_l \left(V_l^\top \left(\ldots \sigma_1 \left(V_1^\top x\right)\right)\right)\right), \tag{16.2}$$

where $W = [V_1, \ldots, V_l, w]$ are the parameters ($V_i \in \mathbb{R}^{n_{i-1} \times n_i}$), each $\sigma_i : \mathbb{R} \mapsto \mathbb{R}$ (acts element-wise) is called as the activation function, and the triplet (σ, l, n), where $\sigma = (\sigma_1, \ldots, \sigma_l), n = (n_0, \ldots, n_l)$, is fixed. The triplet is usually referred to as the architecture and is typically designed from domain knowledge and the learning problem at hand. In case some of the parameters in W are always grounded to zero, then such information is also said to be part of the architecture. Architecture is visualized using figures like 12.19 in Bishop [2006].

The popular choice for the activation function is ReLU: $\sigma(x) \equiv \max(0, x)$. Each function in the composition stack, (16.2), $\sigma(V_i^\top \cdot), i = 1, \ldots, l$, is referred to as a hidden layer. Hence, there are l hidden layers. For convenience, two more layers are defined: x is the input layer, $f_W(x)$ is called the output layer. l is called the depth of the network, and $\max_{i=1,\ldots,l} n_i$ is known as the width of the network. At a later stage we shall discuss some details of using this new model (neural network) to solve a supervised learning problem etc.

Lecture 17

Probabilistic PCA

As in case of clustering in this case of dimensionality reduction too we can design probabilistic models that reflect the underlying generative process. Accordingly we presented the probabilistic PCA model. Please refer section 12.1 in Murphy [2012] for details[1]. The Method of Moments (MM) based derivation from lecture is here: `https://1drv.ms/b/s!Au6Zdrbq2x4ph7c9B0IX4c9Vt2I_-w?e=nIuWvu`. This again showcases the simplicity of MM over MLE (theorem 12.2.2 in Murphy [2012]) for generative models. The advantages of this model are summarized nicely in the beginning of section 12.2 in Bishop [2006]. Most important, is reusability as units in models for (probabilistic) representation learning in the context of supervised learning problems.

[1] You may skip sections 12.1.4-12.1.6.

Lecture 18

Representation Learning along with other Learning Problems

Since a couple of lectures we discussed representation learning with the goal as reconstruction[1]. Now, in some supervised learning applications, it may be the case that one desires to learn appropriate representations. In such a setting, one is not bothered about reconstruction error. What is more important is generalization. Hence the goal in this lecture is to design models for representation learning, which is itself an unsupervised learning problem, that generalize well wrt. the underlying supervised learning problem. Accordingly, we write the ideal goal of Representation learning for supervised set-ups as:

$$\min_{f,g \in \mathcal{G}} \mathbb{E}\left[l\left(Y, f \circ g(X)\right)\right], \tag{18.1}$$

where $\mathcal{G}$ is an appropriate set of representation maps. Here, f is the placeholder for the supervised prediction function being learnt.

We reuse the models from the previous lectures to design powerful models for solving (18.1):

1. As in non-probabilistic dimensionality reduction, we choose $\mathcal{G}$ to be orthognal rotations over a given feature map i.e., $g(x) \equiv L^\top \phi(x)$.

   (a) And, the supervised prediction function by $f(x) = w^\top x$. This leads to

[1] One way to understand the reconstruction objective is that it is "unsupervised".

the following regularized ERM[2] problem:

$$\min_{w\in\mathbb{R}^r, L\in\mathcal{O}_{dr}} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m} l\left(y_i, w^\top L^\top \phi(x_i)\right), \tag{18.2}$$

where $\mathcal{O}_{dr} = \left\{M \in \mathbb{R}^{d\times r} \mid M^\top M = I\right\}$. Such methologies go by the name feature learning.

(b) By using discriminative modeling for supervision like probabilistic logistic regression model, gives the same optimization problem (18.2) with logistic loss, but the interpretation of likelihoods is possible.

2. As in non-probabilistic representation learning, we choose the neural network model to learn the representation. Scalar valued outputs together with squared loss are default for regression and output layer with c neurons, together with logistic loss is default for default for classification. Infact, these models are so popular, and achieve state-of-the-art generalization, that they are typically introduced as models for regression/classification rather than models for representation learning. Analogously, if discrminative modeling is employed[3], then neural network output can be interpreted as likelihoods. All these models form the basics of so-called deep learning.

3. Supervised PCA: refer section 12.5.1 in Murphy [2012]. Regular students need to only understand the definition of this model and the motivation for defining it so.

Like-wise one can talk about representation learning in the context of specific unsupervised learning problems. Here are some pointers for interested students:

1. In case of likelihood estimation:

   (a) Consider an exponential family model, where the sufficient statistics is learned through a neural network. Related to this is energy-based models[4] like Boltzmann machine etc.

   (b) PCA for exponential family models: Collins et al. [2001].

2. In case of novelty detection: (18.2) with only positive class.

3. In case of clustering: mixture of probabilistic PCA models. Refer section 12.1.4 in Murphy [2012].

[2]Interested students may refer eqn. (4) in https://link.springer.com/content/pdf/10.1007/s10994-007-5040-8.pdf for details (in special case $T = 1$ i.e., number of learning tasks is unity).

[3]Objective changes from ERM to MCLE.

[4]If interested please refer https://www.deeplearningbook.org/contents/generative_models.html.

Lecture 19

Stochastic Gradient Descent

A popular framework for efficiently solving the ERM/MLE/MCLE problems encountered in the various models presented in this course is Stochastic Gradient Descent (SGD). One way to understand it is that it is a randomized version of the well-known gradient descent algorithm. However, SGD is not merely a scalable optimization technique. In subsequent lecture it will be shown that it gives a fundamentally different way of solving learning problems, like (3.1,16.1,18.1), without having the need for solving the ERM! We commented that SGD forms the backbone for successful deployment of state-of-the-art deep learning and kernel methods in applications. Please refer sections 14.3, 14.4 in Shalev-Shwartz and Ben-David [2014] for details of SGD and its convergence (you may skip section 14.4.4).

Finally, the perceptron algorithm is nothing but SGD for minimizing risk in case of learning with (unbounded) linear functions + hinge-loss[1].

[1] More precisely, a slightly modified hinge-loss term: $\max(0, -y_i w^\top x_i)$.

Lecture 20

SGD vs ERM

Problems of form (3.1,16.1,18.1), where the objective is to minimize expected value of a function wrt. an unknown likelihood by using iid samples from the same (unknown) likelihood, are called as Stochastic Optimization (SO) problems[1]. In other words, learning in Supervised, Unsupervised settings is essentially the same[2] as solving a Stochastic Optimization problem. Till now, we essentially knew only one paradigm for solving a stochastic optimization problem: minimize the sample based average of the function instead of it's expected value. This is what leads to ERM, MM, MLE, MCLE, etc. This paradigm is referred to as the Sample Average Approximation (SAA). In other word, ERM, MM, MLE, MCLE are all special cases of SAA. It so happens that there is a fundamentally different way to solve SO problems, which is by using SGD. Please refer section 14.5 in Shalev-Shwartz and Ben-David [2014] for details. You may skip sections 14.5.2, 14.5.3, where tighter bounds for other special model classes are presented[3]. In particular, corollary 14.12 provides the following interesting learning bound (for the class of hypothesis functions $g(x) = w^\top \phi(x)$):

$$\mathbb{E}\left[R[\bar{g}_m]\right] \leq R[g^*_{\mathcal{G}}] + \frac{BL}{\sqrt{m}}, \tag{20.1}$$

where the expectation is over the m iid samples, R is the (true) risk functional, $\bar{g}_m$ is the averaged parameter over the m SGD update iterations, $g^*_{\mathcal{G}}$ is the (true

[1] `https://stanford.edu/~jduchi/PCMIConvex/Duchi16.pdf` presents a nice introduction to this problem.

[2] In subsequent lecture, we will see that this is not the case in so-called online settings.

[3] Interested students may read the seminal work: `https://www.cs.cornell.edu/~sridharan/convex.pdf`, where it is shown that if ERM is statistically consistent, then SGD is consistent. However, there are models/inductive-biases/hypothesis-classes where SGD is statistically consistent, whereas ERM is not!

risk) minimizer in the given inductive bias $\mathcal{G}$, B is the distance between the initialization parameter[4] and that with $g^*_{\mathcal{G}}$, L is the Lipshcitz constant of the risk functional. Contrast (20.1), which is the learning bound for SGD, with that in theorem (4.0.1), which is the learning bound for ERM. In-spite of the striking similarity, a key difference is: the former is a deterministic bound, nevertheless about the expected risk with SGD solution, whereas the latter is a high probability bound about the risk with ERM solution. Also, deriving bounds for ERM are a lot more laborious[5] than those for SGD. Finally we commented that in case of ERM, the ERM optimization problem must be solved perhaps using some numerical procedure like gradient descent[6], which leads to an additional error term[7].

We then discussed some practical aspects of applying SGD. Since gradient descent for solving ERM problem uses gradient of loss wrt. all examples at every iteration, and SGD uses one per iteration, a trade-off is achieved by using a few samples per iteration, called as mini-batch. Also, the classical SGD scans the entire training set only once. A pass through training set is called an epoch. In practice, SGD is run for multiple epochs with different random order of samples. Both these tricks lead to the so-called mini-batch SGD, which is the default variant used in practice. Also, though the theorems give a default value for the step-size etc., the hyperparameters like step-size, no. epochs, mini-batch size etc. are typically tuned using validation set procedure[8].

We ended the discussion by providing details of computing the gradient in case of Neural networks, so that SGD can be applied[9]. This is called the Back Propagation algorithm, which is an instance of dynamic programming. Please refer section 20.6 in Shalev-Shwartz and Ben-David [2014] for details and `https://colah.github.io/posts/2015-08-Backprop/` for a nice intuitive explanation.

[4] B is same as W in bounded linear/non-linear models if initial parameter is zero. And in this case, one can show that the complexity of the model turns out to be again BL even in the ERM case!

[5] Hence we skipped them in case of ERM, but did not in case of SGD.

[6] Infact, SGD can also be used to solve the ERM/MLE problems, leading to essentially the same algorithm as SGD for the corresponding SO problem.

[7] Interested students may read the seminal work in Bottou [2010] for other details.

[8] Interested students may refer `http://www.cs.cornell.edu/courses/cs6787/2017fa/Lecture2.pdf` for more details.

[9] `http://www.cs.cornell.edu/courses/cs6787/2017fa/Lecture7.pdf` gives an easy derivation to show why and in which sense does SGD converge for non-convex problems.

Lecture 21

Online Learning

An (unintended) advantage with (classical) SGD is that at every iteration, only one sample is used and the sample can be discarded after updation in that iteration. We argued that this characteristic more closely resembles supervised learning in humans than with ERM i.e., humans experience one event at a time and learn from that experience incrementally. Rarely, the same event reoccurs. It is not the case that multiple events occur (with no learning happening interim of their occurrences) and then the human learns from these experiences. This would be analogous to how ERM works. More importantly, humans are typically evaluated or utilize their predictions even while learning. Accordingly, we defined the online supervised learning framework, where all these characteriztics are encoded nicely. With the following, we qualify the Supervised Learning we talked about earlier as Batch Supervised Learning. Similarly, Batch Unsupervised Learning etc.

21.0.1 Online Supervised Learning

Here examples $(x_1, y_1), (x_2, y_2) \ldots, (x_m, y_m), \ldots$ arrive sequentially. We don't make any assumptions about their generation process. In particular, we DO NOT assume an underlying likelihood $p^*(x, y)$. An online learning algorithm begins with a initial function $g_1 \in \mathcal{G}$, where $\mathcal{G}$ is an appropriate hypothesis-class of functions from $\mathcal{X}$ to $\mathcal{Y}$. When the first example (x_1, y_1) arrives, then the function g_1 is used to make a prediction. The loss $l(y_1, g_1(x_1))$ is then used by the online learning algorithm to choose $g_2 \in \mathcal{G}$. When the second example (x_2, y_2) arrives, then the function g_2 is used to make a prediction. The loss $l(y_2, g_2(x_2))$ is then used by the online learning algorithm to choose $g_3 \in \mathcal{G}$.....and so on.

The quality of an online learning algorithm is typically measured using the cumulative loss incurred over the examples arrived. And then compared with the

cummulative loss incurred by a particular choice, say $h \in \mathcal{G}$. Accordingly, we define the regret of an online algorithm $\mathcal{A}$ wrt. a given $h \in \mathcal{G}$ after m examples as:

$$Regret_{\mathcal{A}}(h, m) \equiv \sum_{i=1}^{m} l\left(y_i, g_i(x_i)\right) - \sum_{i=1}^{m} l\left(y_i, h(x_i)\right).$$

And, overall regret as the regret when compared to the optimal constant hypothesis:

$$Regret_{\mathcal{A}}(m) \equiv \max_{h \in \mathcal{G}} Regret_{\mathcal{A}}(h, m).$$

In the batch setting, $\frac{Regret_{\mathcal{A}}(m)}{m}$ closely resembles the estimation error, and hence a natural definition in online settings.

Instead of setting out to find the best sequence $g_1, \ldots, g_m, \ldots$ that minimizes the regret given data, it is convenient to design online algorithms first and then bound their regret. This should be fine as long as lower bounds of the form as that in theorem 21.10 in Shalev-Shwartz and Ben-David [2014] are known.

It was easy to show that the regret with SGD[1] is $Regret_{\text{SGD}}(m) \leq WL\sqrt{m}$, where W is the bound, $||w|| \leq W$, in bounded linear/non-linear functions and L is Lipschitz constant of loss wrt. the parameter. Please refer section 21.3,21.4 in Shalev-Shwartz and Ben-David [2014] for details.

[1]Infact, the variant of SGD with projection step so that $||w|| \leq W$. This is called as Online Gradient Descent in Shalev-Shwartz and Ben-David [2014].

Lecture 22

Reinforcement Learning: Basics

Using the example of "how infants learn to roll over?", we motivated the need for a new set-up/model in machine learning. This is because humans do not seem to acquire such fundamental skills through examples (either supervised or unsupervised). Accordingly, instead of example-based learning, we introduced the notion of *trial and error* based learning, which will later be formalized as Reinforcement Learning (RL). Informally, we summarized the key characteristics of a reinforcement learning set-up:

1. It is not an example-based learning. Hence, fundamentally very different from both Supervised and Unsupervised Learning.

2. Learning happens by trying various possible actions, which result in rewards (loss or error) i.e., **trail and error**.

3. The motivation for learning is to maximize reward (or minimize loss). In this sense it is similar to supervised learning. Also, rewards are assumed to be stochastic like in supervised learning.

4. Again, like in unsupervised learning, typically RL algorithms directly/indirectly estimation some likelihoods. This is the similarity with unsupervised learning. Like in general online unsupervised learning, the underlying likelihoods may change in a full-fledged RL problem. But most simple is the stationary assumption, where the underlying likelihoods are assumed to be the same at every iteration/step.

5. Like online learning, in RL too the learning agent needs to make sequential decisions and the notion of regret is most natural.

6. However, strikingly different from online supervised learning, the decisions cannot simply try to maximize reward, because perhaps other better rewarding actions are not explored enough. For example, if infant stops trying something different after rolling over, then perhaps it would never learn to crawl! This brings to the most important aspect of RL, which is the trade-off between **exploration-exploitation**.

7. In general RL set-ups, the notion of delayed rewards exists. for e.g., a wrong move in chess will result in negative reward only after many more moves. Such a concept of delayed loss/reward is not present in online supervised learning. The simplest case is that of immediate rewards, which makes it similar to online supervised learning.

8. Another aspect that makes RL fundamentally different from Supervised and Unsupervised Learning is the concept of states. Actions not only result in rewards but also lead to changes in the state of the learning agent (like position of infant).

We then began formally studying restricted versions of the RL set-up, which are easier to analyze. We began with single state, stationary, immediate reward RL, which is formalized as the multi-arm bandit problem. Please refer sections 2-2.1 in Sutton and Barto [2018] for details.

Lecture 23

Multi-arm Bandit Problem

We began formally studying the Bandit problem. Let the set of possible actions be $\{a_1, \ldots, a_k\}$. Let A_t denote the action taken at instant t and R_t be the corresponding reward[1].

We define the value of an action/arm, a_i, as $\mathbb{E}[R_t/A_t = a_i]$ and denote it by $q(a_i)$. Note that by the stationary assumption, the value is independent of the instant, t. We denote the empirical estimate[2] of $q(a_i)$ at instant t by $Q_t(a_i)$. We denote the best arm as the one(s) with the maximum value: $a^* \in \arg\max_{a \in a_1, \ldots, a_k} q(a)$. See also section 2.2 inSutton and Barto [2018].

An algorithm, $\mathcal{A}$, is a data-dependent scheme/policy for choosing the arms to be pulled at every instant based on the Q function. We then defined the regret with an algorithm $\mathcal{A}$ as:

$$regret_{\mathcal{A}}(n) \equiv nq(a^*) - \sum_{i=1}^{k} T_i(n) q(a_i), \tag{23.1}$$

where $T_i(n)$ is the random variable denoting the number of times arm a_i was pulled in first n instants. Obviously, $T_1(n) + \ldots T_k(n) = n$. Typically one is interested in upper bounding the expected regret[3].

Needless to say, if $T_{i^*}(n) = n$, where $a_{i^*} = a^*$, then regret is minimized. However, the identity of this arm is not known and hence learning is relevant. This observation motivates the greedy choice: pick the arm with highest Q_t at t. Unfortunately, such algorithms never explore arms, and will fail to learn the best arm. The other extreme is an algorithm that picks arms at random. It is easy to

[1] Both A_t, R_t are random variables.

[2] One way to estimate is given in equation (2.1) in Sutton and Barto [2018].

[3] If expected regret grows slower than n, then such algorithms are guaranteed to figure out the optimal arm asymptotically.

see that it incurs a very high regret. This leads to our first (provably "correct") algorithm:

ϵ greedy algorithm: Here, the arm with highest Q_t is picked with probability $1-\epsilon$, while at random with probability ϵ.

Another way to have low regret (23.1) is to have $T_i \propto q(a_i)$. Accordingly, we have the so-called soft-max algorithm: where the probability of picking the i^{th} arm is equal to $\frac{e^{Q_t(a_i)}}{\sum_{j=1}^{k} e^{Q_t(a_j)}}$. Both these algorithms have nice regret bounds, but the one that is more popular and insightful is the so-called Upper Confidence Bound (UCB) algorithm. In order to motivate it, we derived the basic bounds that govern the mismatch between Q_t and q: With probability atleast $1-\delta$, we have that[4]

$$q(a_i) \leq Q_s(a_i) + \sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2T_i(s)}}. \tag{23.2}$$

We define the RHS in the above as the Upper Confidence Bound (UCB). Similarly, with probability atleast $1-\delta$, we have that $q(a_i) \geq Q_s(a_i) - \sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2T_i(s)}}$. The RHS in this may be refered to as the Lower Confidence Bound (LCB).

The proof technique we used in lecture is called the Chernoff bounding technique. This is summarized in `https://en.wikipedia.org/wiki/Chernoff_bound#The_generic_bound`. This bound is in terms of moment-generating-functions (mgfs). To further upper bound mgfs, we assumed that the rewards are finite. By the Hoeffding lemma[5], such finitely supported random variables are sub-Gaussian[6], which provides the bound on the mgf. This leads to 23.2.

[4] W.l.o.g., we assume that the rewards are between 0 and 1.

[5] See `https://en.wikipedia.org/wiki/Hoeffding%27s_lemma`.

[6] Interested students may refer `https://ocw.mit.edu/courses/mathematics/18-s997-high-dimensional-statistics-spring-2015/lecture-notes/MIT18_S997S15_Chapter1.pdf`.

Lecture 24

UCB algorithm

Since we know that with high probability, the true mean lies within the LCB and UCB, one can motivate three algorithms for picking the arm: i) the one that chooses an arm with maximum (sample) average. This is the greedy algorithm, which performs no exploration ii) the one that chooses an arm with maximum LCB, which again performs, no exploration. This is because LCB will be higher if either the average is higher or the arm is chosen already many times iii) the one that chooses an arm with maximum UCB, which performs both exploitation and exploration. This is because UCB will be higher if either the average is higher or the arm is chosen a very few times.

Given that UCB is a good strategy, the crucial question is the choice of δ in (23.2). It is clear that during initial iterations, high delta would simple mean arbitrary choice for arms because the variance in (23.2) will be too high. Accordingly, we choose $\delta = \frac{1}{m^\alpha}$, where $\alpha > 1$ is a hyperparameter. Please refer theorem 1 in Auer et al. [2002] for details of regret bound with the UCB algorithm or this handwritten-notes: see "TechnicalDerivations− >UCB regret bound" in `https://1drv.ms/o/s!Au6Zdrbq2x4ph7JQUbky8SW6ygknAg`[1].

The most interesting take homes from this regret analysis are:

1. The regret after m rounds is bounded by $O(\log(m))$, which is in some sense is a negligible increase. Less interestingly, this also shows that UCB figures out the best arm(s) asymptotically.

2. The bound on regret is lower, if the margin between the value of the best arm(s) and the rest are higher. This is indeed insightful and illustrates the goodness of this bound.

[1]Same as the version in `https://www.cse.iitb.ac.in/~shivaram/teaching/old/cs747-a2018/resources/ucb-regret.pdf`.

Though Bandits do not expose all aspects of a full RL problem, it does highlight the important explore-exploit trade-off, which makes RL a unique and interesting problem to study. Interested students may study Sutton and Barto [2018], which is an excellent book on basics of RL.

Lecture 25

Strong and Weak Learning

Till now, we talked about three fundamental learning problems/settings in machine learning: SL (Supervised Learning), UL (Unsupervised Learning), RL (Reinforcement Learning). The key quantity of interest in batch SL,UL is the generalization error and that in online SL,UL, and RL is the regret. In some sense both regret and generalization reflect the performance of an algorithm wrt. their performance in terms of *learning* alone.

There are many other main aspects to learning than merely generalization error/regret. For example, computational complexity, interpretability, privacy, robustness to noise and adversaries etc. The fundamental trade-offs between each of these and learning has been studied well.

An amazing result in the study of trade-off between learning and computational complexity is AdaBoost, which shows that computational effort has almost no bearing on the so-called "strength of learning"! We shall present details of AdaBoost, which can also be understood as an alternative to ERM/SGD, in the subsequent lecture. For now, we shall introduce formally the notions of strong/weak learning in the context of batch SL.

A set of candidate functions for the Bayes optimal is defined as the Concept class. The combination of a model (i.e., loss+inductive-bias) together with an algorithm like ERM/SGD is defined as a learner/learning-algorithm.

The bound in theorem 4.0.1 shows that ERM achieves Bayes consistency if the inductive bias is same as the concept class, provided the complexity of the corresponding model is finite. In such a situation, we say the learner (in this case defined by ERM+concept class) is a strong learner and the concept class is strongly learnable[1].

[1]In the sense that there exists alteast one strong learner for the concept class. Note that if the

A relaxed version of this is the so-called weak learning. To define this formally, let us assume a Binary classification setting with 0-1 loss and assume that the risk with Bayes optimal is zero. In such a special case, strong learning condition is same as: for any $\delta \in [0,1], \epsilon > 0$, and high enough samples m, with probability atleast $1-$ (over the samples), misclassification probability with the strong learner, g_m^s, which is $P\left[Y \neq g_m^s(X)\right]$ is $\leq \epsilon$. Now we define γ-weak learner, g_m^γ, if $\exists\ \delta_0 < 1,\ \exists\ \epsilon_0 \leq 0.5 - \gamma$ such that with probability atleast $1 - \delta_0$, $P\left[Y \neq g_m^\gamma(X)\right] \leq \epsilon_0$. If a γ-weak learner exists for a concept class, then it is called γ-weak learnable.

The intuition behind these definitions are: weak learners can be trained with cheap computational effort (this is indeed true), whereas there may be some (difficult) concept classes where weak learners are computational efficient whereas strong learners are not. A Godel prize winning seminal work Freund and Schapire [1997] is that the later statement is false! In other words, computationally efficient weak learning is possible if and only if computationally efficient strong learning is possible!!

Please go through example 10.1 in Shalev-Shwartz and Ben-David [2014] to understand weak learning definition. A popular example of a weak learner (over R^n input space) is $\mathcal{G}_0$ together with ERM, where

$$\mathcal{G}_0 \equiv \{g : \mathbb{R}^n \mapsto \{-1, 1\} \mid \exists\ i \in 1, \ldots, n,\ \theta_i \in \mathbb{R},\ \ni\ \ g(x) = \text{sign}(x_i - \theta_i)\} \tag{25.1}$$

is the set of so-called Decision Stumps. Section 10.1.1 in Shalev-Shwartz and Ben-David [2014] shows that ERM over $\mathcal{G}_0$ can be performed in linear time (efficiently). In the subsequent lecture, we will show that by training such weak learners almost constant number of times will give strong learners!

concept class's complexity is not finite, then theorem 4.0.1 does not guarantee that the concept class is strongly learnable.

Lecture 26

Bagging, Boosting and Decision Trees

If one needs to graduate to strong learning from weak learning, then there are two gaps that need to be bridged:

Variance: There are smart sampling techniques that can be used to reduce the variance (i.e., increase the confidence). The most popular is bagging. The idea is to create so-called bootstrap datasets, which are nothing but m-sized sets, k in number, which are obtained by sampling with replacement from the given m-sized dataset. The same learner is then trained with these k-sets leading to k prediction functions. The final prediction function is defined as the average of these.

Bias: Reducing $\epsilon_0 \leq \frac{1}{2} - \gamma$ to zero is not as simple as reducing variance. This is because of the approximation/modeling error between the concept class and the inductive bias in the weak learner. Note that the approximation error could be as large as $\frac{1}{2} - \gamma$ itself. Interestingly, this gap can be bridged using the so-called Boosting techniques. These are iterative techniques, which at each iteration train the given weak learner with various distributions (weights) over the training dataset. The final prediction function is defined as a the weighted sum (or majority vote) with these trained weak learners. The intuition is that the trained weak learners are expected to be strong learners locally i.e., in specific subsets of the inputspace. And the final combined (voted) predictor will be strong globally (i.e., everywhere inside the inputspace).

Please refer sections 10.2, 10.4 in Shalev-Shwartz and Ben-David [2014] for details of a popular boosting algorithm called AdaBoost. Interested students may

also read section 10.3 and further study Schapire and Freund [2012], which is a great book that is entirely devoted to boosting.

Interestingly, decision stumps not only lead to computationally efficient (strong) learners (via AdaBoost), but also are attractive for their interpretability. In some sense, the most interpretable learners are the decision trees, which are nothing but multiple decision stumps applied recursively. These are called as decision trees. Please refer section 18.2 in Shalev-Shwartz and Ben-David [2014] for details.

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