**About this class**

**Theme** We introduce the learning problem as the problem of function approximation from sparse data. We define the key ideas of loss functions, empirical error and generalization error. We then introduce the Empirical Risk Minimization approach and the two key requirements on algorithms using it: well-posedness and consistency. We then describe a key algorithm – Tikhonov regularization – that satisfies these requirements.

**Math Required** Familiarity with basic ideas in probability theory.
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Plan

- Learning as function approximation
- Empirical Risk Minimization
- Generalization and Well-posedness
- Regularization
- Appendix: Sample and Approximation Error
We assume that $X$ and $Y$ are two sets of random variables. We are given a training set $S$ consisting $n$ samples drawn i.i.d. from the probability distribution $\mu(z)$ on $Z = X \times Y$:

$$(x_1, y_1), \ldots, (x_n, y_n)$$

that is $z_1, \ldots, z_n$

We will make frequent use of the conditional probability of $y$ given $x$, written $p(y|x)$:

$$\mu(z) = p(x, y) = p(y|x) \cdot p(x)$$

It is crucial to note that we view $p(x, y)$ as fixed but unknown.
Probabilistic setting

Tomaso Poggio
The Learning Problem and Regularization
The hypothesis space $\mathcal{H}$ is the space of functions that we allow our algorithm to provide. For many algorithms (such as optimization algorithms) it the space the algorithm is allowed to search. As we will see, it is often important to choose the hypothesis space as a function of the amount of data available.
The basic goal of **supervised learning** is to use the training set $S$ to “learn” a function $f_S$ that looks at a new $x$ value $x_{new}$ and predicts the associated value of $y$

$$y_{pred} = f_S(x_{new})$$

If $y$ is a real-valued random variable, we have **regression**. If $y$ takes values from an unordered finite set, we have **pattern classification**. In two-class pattern classification problems, we assign one class a $y$ value of 1, and the other class a $y$ value of $-1$. 
In order to measure goodness of our function, we need a loss function $V$. In general, we let $V(f, z) = V(f(x), y)$ denote the price we pay when we see $x$ and guess that the associated $y$ value is $f(x)$ when it is actually $y$. 
For regression, the most common loss function is square loss or L2 loss:

\[ V(f(x), y) = (f(x) - y)^2 \]

We could also use the absolute value, or L1 loss:

\[ V(f(x), y) = |f(x) - y| \]

Vapnik’s more general \( \epsilon \)-insensitive loss function is:

\[ V(f(x), y) = (|f(x) - y| - \epsilon)_+ \]
For binary classification, the most intuitive loss is the 0-1 loss:

$$V(f(x), y) = \Theta(-yf(x))$$

where $\Theta(-yf(x))$ is the step function. For tractability and other reasons, we often use the hinge loss (implicitly introduced by Vapnik) in binary classification:

$$V(f(x), y) = (1 - y \cdot f(x))_+$$
There is an unknown **probability distribution** on the product space \( Z = X \times Y \), written \( \mu(z) = \mu(x, y) \). We assume that \( X \) is a compact domain in Euclidean space and \( Y \) a closed subset of \( \mathbb{R} \). The **training set** \( S = \{(x_1, y_1), \ldots, (x_n, y_n)\} = \{z_1, \ldots, z_n\} \) consists of \( n \) samples drawn i.i.d. from \( \mu \).

\( \mathcal{H} \) is the **hypothesis space**, a space of functions \( f : X \rightarrow Y \).

A **learning algorithm** is a map \( L : Z^n \rightarrow \mathcal{H} \) that looks at \( S \) and selects from \( \mathcal{H} \) a function \( f_S : x \rightarrow y \) such that \( f_S(x) \approx y \) in a **predictive way**.
Empirical error, generalization error, generalization

Given a function \( f \), a loss function \( V \), and a probability distribution \( \mu \) over \( Z \), the expected or true error of \( f \) is:

\[
I[f] = \mathbb{E}_z V[f, z] = \int_Z V(f, z) d\mu(z)
\]

which is the expected loss on a new example drawn at random from \( \mu \).

We would like to make \( I[f] \) small, but in general we do not know \( \mu \).

Given a function \( f \), a loss function \( V \), and a training set \( S \) consisting of \( n \) data points, the empirical error of \( f \) is:

\[
I_S[f] = \frac{1}{n} \sum V(f, z_i)
\]
A very natural requirement for $f_S$ is distribution independent generalization

$$\forall \mu, \lim_{n \to \infty} |I_S[f_S] - I[f_S]| = 0 \text{ in probability}$$

In other words, the training error for the solution must converge to the expected error and thus be a “proxy” for it. Otherwise the solution would not be “predictive”.

A desirable additional requirement is **universal consistency**

$$\forall \epsilon > 0 \lim_{n \to \infty} \sup_{\mu} \mathbb{P}_S \left\{ I[f_S] > \inf_{f \in \mathcal{H}} I[f] + \epsilon \right\} = 0.$$

*Remark:* For some of the results to be mentioned the requirement of uniform convergence must be added in both definitions.
Let \( \{X_n\} \) be a sequence of bounded random variables. We say that

\[
\lim_{n \to \infty} X_n = X \text{ in probability}
\]

if

\[
\forall \varepsilon > 0 \lim_{n \to \infty} P\{|X_n - X| \geq \varepsilon\} = 0.
\]

or

if for each \( n \) there exists a \( \varepsilon_n \) and a \( \delta_n \) such that

\[
P \{|X_n - X| \geq \varepsilon_n\} \leq \delta_n,
\]

with \( \varepsilon_n \) and \( \delta_n \) going to zero for \( n \to \infty \).
Given a training set $S$ and a function space $\mathcal{H}$, empirical risk minimization (Vapnik introduced the term) is the algorithm that looks at $S$ and selects $f_S$ as

$$f_S = \arg \min_{f \in \mathcal{H}} I_S[f]$$

The solution to this problem does not in general exhibit generalization and the problem may be ill-posed, depending on the choice of $\mathcal{H}$. If the minimum does not exist we can work with the infimum. Notice: *For ERM generalization and consistency are equivalent*
For the solution of ERM to be useful in the context of learning, the solution must

- “generalize”
- exist, be unique and be “stable” (well-posedness).
Here is a graphical example for generalization: given a certain number of samples...
suppose this is the “true” solution...
... but suppose ERM gives this solution!
How can I guarantee that for a sufficient number of examples the ERM solution will converge to the true one?
Uniform Glivenko-Cantelli Classes

\( \mathcal{L} = \{ \mathcal{H} \circ V \} \) is a (weak) uniform Glivenko-Cantelli (uGC) class if

\[
\forall \varepsilon > 0 \lim_{n \to \infty} \sup_{\mu} \mathbb{P}_{S} \left\{ \sup_{\ell \in \mathcal{L}} |l[\ell] - l_S[\ell]| > \varepsilon \right\} = 0.
\]

**Theorem** [Vapnik and Červonenkis (71), Alon et al (97), Dudley, Giné, and Zinn (91)]

A necessary and sufficient condition for consistency of ERM is that \( \mathcal{L} \) is uGC.

Thus, as we will see later, a proper choice of the hypothesis space \( \mathcal{H} \) ensures generalization of ERM (and consistency since for ERM generalization is necessary and sufficient for consistency and vice versa). We will be exploring the uGC definition (and equivalent definitions) in detail in 9.520.
ERM is in general an ill-posed problem. It can be made well-posed by an appropriate choice of $\mathcal{H}$. As we will see later, well-posedness is mainly used to mean stability of the solution: $f_S$ depends continuously on the training set $S$. In particular, changing one of the training points should affect less and less the solution as $n$ goes to infinity.
A problem is **well-posed** if its solution:

- exists
- is unique
- depends continuously on the data (e.g. it is stable)

A problem is **ill-posed** if it is not well-posed.
Here is a graphical example for stability: given 10 samples...
...we can find the smoothest interpolating polynomial (which degree?).
But if we perturb the points slightly...
...the solution changes a lot.
If we restrict ourselves to degree two polynomials...
...the solution varies only a small amount under a small perturbation.
The basic idea of regularization (originally introduced by Tikhonov independently of the learning problem) is to restore well-posedness of ERM by constraining the hypothesis space $\mathcal{H}$. The direct way – minimize the empirical error subject to $f$ in a ball in an appropriate $\mathcal{H}$ – is called Ivanov regularization. The indirect way is Tikhonov regularization (which is not ERM).
Ivanov and Tikhonov Regularization

ERM finds the function in \((\mathcal{H}, \| \cdot \|)\) which minimizes

\[
\frac{1}{n} \sum_{i=1}^{n} V(f(x_i), y_i)
\]

which in general – for arbitrary hypothesis space \(\mathcal{H}\) – is \textit{ill-posed}.

Ivanov regularizes by finding the function that minimizes

\[
\frac{1}{n} \sum_{i=1}^{n} V(f(x_i), y_i)
\]

while satisfying

\[
\|f\|^2 \leq A.
\]

Tikhonov regularization minimizes over the hypothesis space \(\mathcal{H}\), for a fixed positive parameter \(\gamma\), the regularized functional

\[
\frac{1}{n} \sum_{i=1}^{n} V(f(x_i), y_i) + \gamma \|f\|^2_K,
\]

where \(\|f\|_K\) is the norm in \(\mathcal{H}\) – the Reproducing Kernel Hilbert Space (RKHS), defined by the kernel \(K\).
Well-posed and Ill-posed problems

Hadamard introduced the definition of ill-posedness. Ill-posed problems are typically inverse problems. As an example, assume $g$ is a function in $Y$ and $u$ is a function in $X$, with $Y$ and $X$ Hilbert spaces. Then given the linear, continuous operator $L$, consider the equation

$$g = Lu.$$ 

The direct problem is to compute $g$ given $u$; the inverse problem is to compute $u$ given the data $g$. In the learning case $L$ is somewhat similar to a “sampling” operation and the inverse problem becomes the problem of finding a function that takes the values

$$f(x_i) = y_i, \ i = 1, \ldots, n$$

The inverse problem of finding $u$ is well-posed when

- the solution exists,
- is unique and
- is stable, that is depends continuously on the initial data $g$. 
As we will see in future classes

- Tikhonov regularization ensures well-posedness eg existence, uniqueness and especially *stability* (in a very strong form) of the solution
- Tikhonov regularization ensures generalization
- Tikhonov regularization is closely related to – but different from – Ivanov regularization, eg ERM on a hypothesis space $\mathcal{H}$ which is a ball in a RKHS.
• In the next class we will introduce RKHS: they will be the hypothesis spaces we will work with.
• We will also derive the solution of Tikhonov regularization.
In addition to the hypothesis space $\mathcal{H}$, the space we allow our algorithms to search, we define...

The **target space** $\mathcal{T}$ is a space of functions, chosen a priori in any given problem, that is assumed to contain the “true” function $f_0$ that minimizes the risk. Often, $\mathcal{T}$ is chosen to be all functions in $L_2$, or all differentiable functions. Notice that the “true” function if it exists is defined by $\mu(z)$, which contains all the relevant information.
Sample Error (also called Estimation Error)

Let \( f_\mathcal{H} \) be the function in \( \mathcal{H} \) with the smallest true risk. We have defined the generalization error to be \( l_S[f_S] - l[f_S] \). We define the sample error to be \( l[f_S] - l[f_\mathcal{H}] \), the difference in true risk between the best function in \( \mathcal{H} \) and the function in \( \mathcal{H} \) we actually find. This is what we pay because our finite sample does not give us enough information to choose to the “best” function in \( \mathcal{H} \). We’d like this to be small. Consistency – defined earlier – is equivalent to the sample error going to zero for \( n \to \infty \).

A main goal in classical learning theory (Vapnik, Smale, ...) is “bounding” the generalization error. Another goal – for learning theory and statistics – is bounding the sample error, that is determining conditions under which we can state that \( l[f_S] - l[f_\mathcal{H}] \) will be small (with high probability).

As a simple rule, we expect that if \( \mathcal{H} \) is “well-behaved”, then, as \( n \) gets large the sample error will become small.
Let $f_0$ be the function in $\mathcal{T}$ with the smallest true risk. We define the **approximation error** to be $l[f_{\mathcal{H}}] - l[f_0]$, the difference in true risk between the best function in $\mathcal{H}$ and the best function in $\mathcal{T}$. This is what we pay because $\mathcal{H}$ is smaller than $\mathcal{T}$. We’d like this error to be small too. In much of the following we can assume that $l[f_0] = 0$. We will focus less on the approximation error in 9.520, but we will explore it.

As a simple rule, we expect that as $\mathcal{H}$ grows bigger, the approximation error gets smaller. If $\mathcal{T} \subseteq \mathcal{H}$ – which is a situation called the *realizable setting* – the approximation error is zero.
We define the error to be \( l[f_S] - l[f_0] \), the difference in true risk between the function we actually find and the best function in \( \mathcal{T} \). We'd really like this to be small. As we mentioned, often we can assume that the error is simply \( l[f_S] \).

The error is the sum of the sample error and the approximation error:

\[
l[f_S] - l[f_0] = (l[f_S] - l[f_H]) + (l[f_H] - l[f_0])
\]

If we can make both the approximation and the sample error small, the error will be small. There is a tradeoff between the approximation error and the sample error...
The Approximation/Sample Tradeoff

It should already be intuitively clear that making $\mathcal{H}$ big makes the approximation error small. This implies that we can (help) make the error small by making $\mathcal{H}$ big. On the other hand, we will show that making $\mathcal{H}$ small will make the sample error small. In particular for ERM, if $\mathcal{H}$ is a uGC class, the generalization error and the sample error will go to zero as $n \to \infty$, but how quickly depends directly on the “size” of $\mathcal{H}$. This implies that we want to keep $\mathcal{H}$ as small as possible. (Furthermore, $\mathcal{T}$ itself may or may not be a uGC class.) Ideally, we would like to find the optimal tradeoff between these conflicting requirements.