# Introduction:

深度神经网络作为机器学习的一个分支，已经越来越被科研工作者们所重视，许多在传统理论的上无法解决的问题，应用深度神经网络都能得到很好的解决。深度神经网络的基本结构是通过再输入节点和输出节点之间建立多层的参数结构进行连接，很明显，当深度神经网络的层数够多，所获得的对应的数学函数就可以极大的逼近输入信号和输出信号之间的自然关系。之所以深度神经网络如此申请，目前有两种观点[1]，一种观点认为深度神经网络是向量空间中连续函数的通用逼近器，另一种观点提出了，尽管深度神经网络需要大量的参数，但是使用误差反向传播机制都能够得到有效的训练。

虽然可以通过反向传播逐步使得深度神经网络的参数收敛，但是目前深度神经网络仍然有一些明显的缺陷：

1)如果训练集的数据量不够大时，神经网络的精度就比较差[2]；

2)即使训练集的数据量足够大，如果训练集的质量不够高也会导致神经网络的泛化能力比较差，即出现过拟合[3][4]。

3)目前还没有明确的方法来有效的寻找深度神经网络中的超参数。

之所以深度神经网络会有上述的这些问题，是因为深度神经网络就像以一个“黑盒子” 一样，因此有必要给出一种有效的理论来对深度神经网络的功能给出解释。实际上，深度神经网络是由有向无环图组成的，而GSP可以将傅里叶分析扩展到任何使用图来描述的拓扑域，因此本文提出使用图信号处理（GSP）的方法来监视深度神经网络的训练过程中间层的表示，通过GSP检测深度神经网络发生过拟合的情况，并试图发现深度神经网络性能达到最佳的过程中的特征变化，从而为深度神经网络的构建和训练提供指导。

# Background:

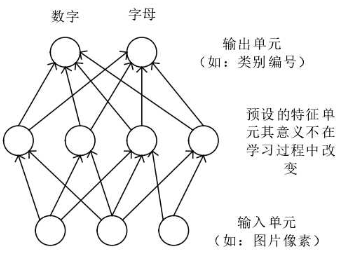
In this section the various aspects of the background to the project will be presented.

## background of GSP

Data is all around us, and massive amounts of it. Almost every aspect of human life is now being recorded at all levels: from the marking and recording of processing inside the cells starting with the advent of fluorescent markers, to our personal data through health monitoring devices and apps, financial and banking data, our social networks, mobility and traffic patterns, marketing preferences, fads, and many more. The complexity of such networks [5] and interactions means that the data now reside on irregular and complex structures that do not lend themselves to standard tools.Graphs offer the ability to model such data and complex interactions among them. For example, users on Twitter can be modeled as nodes while their friend connections can be modeled as edges. This paper explores adding attributes to such nodes and modeling those as signals on a graph; for example, year of graduation in a social network, temperature in a given city on a given day in a weather network, etc. Doing so requires us to extend classical signal processing concepts and tools such as Fourier transform, filtering, and frequency response to data residing on graphs. It also leads us to tackle complex tasks such as sampling in a principled way. The field that gathers all these questions under a common umbrella is graph signal processing (GSP) [6], [7]. While the precise definition of a graph signal will be given later in the paper, let us assume for now that a graph signal is a set of values residing on a set of nodes. These nodes are connected via (possibly weighted) edges. As in classical signal processing, such signals can stem from a variety of domains; unlike in classical signal processing, however, the underlying graphs can tell a fair amount about those signals through their structure. Different types of graphs model different types of networks that these nodes represent. Typical graphs that are used to represent common realworld data include Erdo˝s–Rényi graphs, ring graphs, random geometric graphs, small-world graphs, power-law graphs, nearest-neighbor graphs, scale-free graphs, and many others. These model networks with random connections (Erdoo˝s– Rényi graphs), networks of brain neurons (small-world graphs), social networks (scale-free graphs), and others. As in classical signal processing, graph signals can have properties, such as smoothness, that need to be appropriately defined. They can also be represented via basic atoms and can have a spectral representation. In particular, the graph Fourier transform allows us to develop the intuition gathered in the classical setting and extend it to graphs; we can talk about the notions of frequency and bandlimitedness, for example. We can filter graph signals. They can be sampled, a notoriously hard problem; with GSP, one gains access to principled tools mimicking the classical ones. We can denoise graph signals, we can learn their underlying structure, we can model them. If the graphs cannot be directly observed, we can also learn their structure from data.

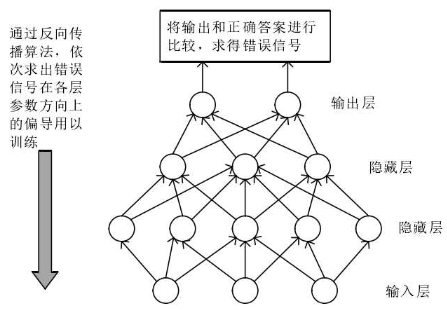
## history or DeepNeural Network

作为一个非常有效的数学工作，机器学习算法，尤其是神经网络早在上个实际的60年代就已经出现，当时的科学家以生物神经网络为原型，提出了第一代神经网络模型，当时被称为感知器[8]，第一代神经网络的特点是其特征需要人工事先输入，在进行模式识别时，是基于特征权重的。它的局限性在于对具体任务的处理效果不佳。因此第一代神经网络的使用范围往往极为有限，第一代神经网络感知器模型如下。



Marvin Minsky 和 Seymour Papert 于1969年[9]探讨了第一代神经网络没有能力处理异或逻辑问题的缺点，这使得其他研究者们对于神经网络越来越没有信心，因此，自1970年起，神经网络的研究和发展进入了一个低潮期。

1982年，物理学家John Hopfiled[10] 提出了一种新的神经网络模型，被称为 Hopfield 模型，并首次提出了能量的定义。Hopfiled 模型具有很强的容错性能，并能够从不完整或失真的数据图像中重构出完整的数据图像。即第一代神经网络模型之后，Hopfield 的模型被称为第二代神经网络，与初代感知器不同的是，Hopfield 模型不再使用预设的特征，而是由算法在训练过程中自动适应，因此就解决了使用范围狭窄的问题。在训练的适合，这类神经网络采用了一种反向传播算法[11]，从输入层将样本的误差反向传播到输入层，网络的权值在传播的过程中不断的调整，提高神经网络对于样本的似然度。同时，虽然隐含层可以加强网络的表达能力，但是它的引入也使得网络的复杂度提高了。第二代神经网络模型如图所示。



与第一代神经网络相比，第二代虽然能够处理较多的问题，但是还是由明显的缺点：1）监督学习是他唯一的用途，而且在训练数据时要使用标号。绝大多数的真实环境中的数据是没有标号的。（2）训练时间很长，特别是隐含层特别多的情况下，但是如果减少了隐含层就会降低精度。（3）反向传播算法容易陷入局部最优解。因此神经网络的发展又进入了第二个低谷。

直到时间来到了2016年，Hinton[12]首次提出了深度网络和深度学习的理论[13]，并发表在了《科学》杂志上，由此引起了人们对于深度学习的注意。深度学习架构是由多层非线性运算单元构成，能够学习表示高阶抽象概念的复杂函数，从低到高的过程中，底层输出作为高层输入。通过多次的输入数据学习，可以得到它的结构信息的高阶特征表示，用于分类、回归和信息检索等特定问题中。深度学习的诞生给予了研究人工智能的新希望[14]。

不过目前的研究水平，人们还不能掌握每层学习到的特征是什么样的，本设计提出了采用GSP方法来分析深度神经网络中间层的特征，从而为深度神经网络的精度和性能提供依据。

## GSP application

网络或者说图的应用无论是在科研或者是日常生活中都非常常见，比如社交网络，生物网络，通信网络等等。而近几年，随着人工智能的发展，深度神经网络也随之兴起。然而深度学习一直以来都是以“黑盒子”的形态呈现在研究人员的面前，尽管最近有不少深度神经网络结构在各个领域都取得了前所未有的成就，比如图像分类领域，深度神经网络的精度能够达到70%以上(top1)和90%以上(top5)，这样的精度已经达到甚至超过了人类的分类能力。然而，却没有明确的理论支持为什么深度神经网络能够达到这样的精度，实际上，大部分神经网络的构建或者创新往往都有猜测的成分，因此急需一种手段深入神经网络内部去寻找某些可以衡量或者指导神经网络的指标。

深度神经网络本质是有向无环图，其每个节点表示一个可以与标签关联的数据节点，并且通过连接不同节点边以及给每个边分配各自的权重形成图。既然是图，必然遵循图论，因此图论相关的方法在深度神经网络的应用中具有非常重要的指导意义。图信号处理（GSP）是图论中非常重要的工具之一，GSP可以对图的不同节点进行不同形式的处理、过滤等等操作。当数据标签在图上作为信号呈现时，图信号正则化技术可以用于标签估计的过程中，从而优化分类和半监督学习问题中未知标签的预测。

the GSP framework can also be used to design architectures to analyze or classify whole graph signals that originally live on irregular structures. In particular, the GSP toolbox has been extensively used to extend convolutional deep learning techniques to data defined on graphs. The convolutional neural network paradigm has been generalized with help of GSP elements for the extraction of feature descriptors for 3-D shapes [15], [16]. A localized spectral network architecture leveraging on localized vertexfrequency analysis has also been proposed in [17], and the use of heat kernels defined in the graph spectral domain has been developed in [18]. While the previous works mostly address the analysis of 3-D shapes, convolutional neural networks (CNNs) can actually be extended to many other signals in high-dimensional irregular domains, such as social networks, brain connectomes, or words embedding, by reformulation in the context of spectral graph theory. Here, the GSP framework leads to the development of fast localized convolutional filters on graphs [19] along with adapted pooling operators [20]. Unsurprisingly, deep network architectures for graphs signals have been actually tested in various applications domains, such as chemical molecule properties prediction [21], classification tasks on social networks [22], autism spectrum disorder classification [23], or traffic forecasting [24].

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