Notes on Machine Learning & Deep Learning

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Contents

1 Introduction

In this section, we briefly introduce some useful aspects of machine learning (ML), some basic concepts in information theory, and two statistical estimators for ML models.

1.1 Machine learning

▷ Domingos, "A few useful things to know about machine learning" (2012).

$$\text{Learning} = \text{Representation} + \text{Evaluation} + \text{Optimization}$$

▷ Machine learning: "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E.", by Tom M. Mitchell. Mainly concern the **opertional definition**, rather than defining in cognitive terms. This approach is **data driven**, instead of knowledge (logic) or statistics driven.
▷ Problems/Tasks: Three categories: Supervised, unsupervised, & reinforcement learning. Briefly divided into: Classification, regression, clustering, dimension reduction
▷ Hyperparameters: controls the representation capacity of the model (linear model, NN etc). In Bayesian statistics, hyperparameters are just the parameters in the prior belief. For NN, they include number of layers etc.

1.2 Information theory

Ref: [Goodfellow] Section 3.13. Read also [Goodfellow] Sections 3.1 for the reasons why **probability models** are used in statistical learning & deep learning.

1.2.1 Self-information

For only a single outcome

$$I(x) = -\log P(x)$$

(1) Likely events should have low information content
(2) Less likely events should have higher information content
(3) Independent events should have **additive** information

1.2.2 Shannon entropy

To quantify the amount of uncertainty in an entire probability distribution, use the Shannon entropy

$$H(x) = \mathbb{E}_{x\sim P}[I(x)] = -\mathbb{E}_{x\sim P}[\log P(x)]$$

which gives a lower bound on the number of bits needed on average to encode symbols drawn from a distribution P.

1.2.3 KL (Kullback-Leibler) divergence

Defined as

$$D_{\mathrm{KL}}(P||Q) = \mathbb{E}_{x\sim P}[\log P(x) - \log Q(x)]$$

which is the extra amount of information needed to send a message containing symbols drawn from P, when we use a code that was designed to minimize the length of messages drawn from Q. It is non-negative, and it is zero iff P and Q are identical distribution. Also $D_{\mathrm{KL}}(P||Q) \neq D_{\mathrm{KL}}(Q||P)$.

▶ *Proof* (Non-negativity of D_{KL}): Using Jensen's inequality $\mathbb{E}[f(x)] \geq f(\mathbb{E}[x])$ for a convex function $f(x)$,

$$\begin{aligned} D_{\mathrm{KL}}(P||Q) &= -\int dx P \log \frac{Q}{P} \\ &\geq -\log\left[\int dx P \cdot \frac{Q}{P}\right] = 0 \end{aligned}$$

where we take $f(x) = -\log x$. Note: A more rigirious derivation needs to concern about the set A such that $P(x) > 0, \forall x \in A$. See [Murphy] Theorem 2.8.1. ◀

▶ *Jensen's inequality*: For any convex function $f(x)$, we have

$$\sum_{i=1}^{n} \lambda_i f(x_i) \geq f\left(\sum_{i=1}^{n} \lambda_i x_i\right)$$

where $\lambda_i \geq 0$ and $\sum_i \lambda_i = 1$. This is clearly true for $n = 2$ by definition of convexity, and can be proved by induction for $n > 2$. ◀

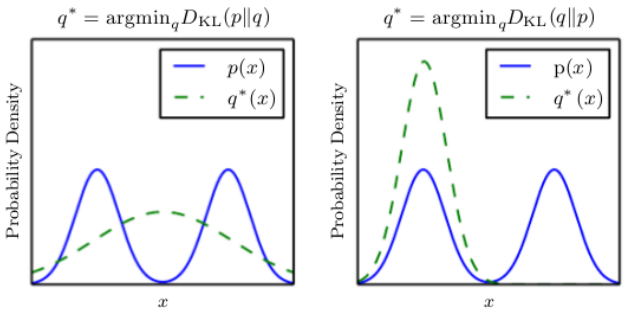


Figure 1: [Goodfellow] Fig. 3.6. (Left, **mass covering**) The effect of minimizing $D_{\mathrm{KL}}(p||q)$, such that a $q(x)$ with high probability overlap with $p(x)$ is selected. (Right, **mode collapse** or **mode seeking**) The effect of minimizing $D_{\mathrm{KL}}(q||p)$, such that a $q(x)$ that has low probability where $p(x)$ has low probability is selected. Reason: For some x, $q(x) \to 0$ and $p(x) \to 1$, then $q(x) \log \frac{q(x)}{p(x)} \to 0$, hence vanishing contribution to $D_{\mathrm{KL}}(q||p)$; while $q(x) \to 1$ and $p(x) \to 0$, then $q(x) \log \frac{q(x)}{p(x)} \to +\infty$, hence large contribution to $D_{\mathrm{KL}}(q||p)$.

1.3 Statistical estimators

Ref: [Goodfellow] Sections 3.11 & 5.6

1.3.1 Bayesian Statistics

▷ Conditional Probability: Defined as

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

▷ Bayes' Rule: Given by

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} = \frac{P(B|A)P(A)}{\sum_{a \in A} P(B|A)P(A)}$$

where the second equality utilizes $P(B) = \sum_{a \in A} P(B \cap A)$.

▷ Bayesian Inference:

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)} \quad \text{or} \quad \text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{evidence}}$$

Prior and *posterior* are probability distributions for our *beliefs* before and after revealing the *evidence*. The likelihood $P(D|\theta)$ is the probability of seeing the evidence as generated by a prior model $P(\theta)$ with parameter θ. Starting with the model θ, our posterior belief is *adjusted* by the evidence D to be $P(\theta|D)$.

1.3.2 MLE (Maximum likelihood estimation)

Maximum likelihood estimator $\hat{\theta}$ for θ is defined as

$$\begin{aligned}
\hat{\theta}_{\text{ML}} &= \arg\max_{\theta} p_{\text{model}}(\{x^{(i)}\}; \theta) \\
&= \arg\max_{\theta} \prod_{i=1}^{m} p_{\text{model}}(x^{(i)}; \theta) \\
&= \arg\max_{\theta} \sum_{i=1}^{m} \log p_{\text{model}}(x^{(i)}; \theta) \\
&= \arg\max_{\theta} \mathbb{E}_{x \sim \hat{p}_{\text{data}}} \log p_{\text{model}}(x; \theta) \\
&= \arg\min_{\theta} D_{\text{KL}}(\hat{p}_{\text{data}} || p^{(\theta)}_{\text{model}}) \\
&= \arg\min_{\theta} \mathbb{E}_{x \sim \hat{p}_{\text{data}}} [\log \hat{p}_{\text{data}}(x) - \log p_{\text{model}}(x; \theta)]
\end{aligned}$$

► *Aside* [(Point) Estimator or Statistic]: Let $\{x^{(i)}\}$ be a set of m i.i.d. data points. An estimator $\hat{\theta}_m$ of the parameter θ is any function of the data:

$$\hat{\theta}_m = g(\{x^{(i)}\})$$

Bias: of an estimator is defined as

$$\text{bias}(\hat{\theta}_m) = E(\hat{\theta}_m) - \theta$$

where the expectation is over the data (seen as samples from a random variable) and θ is the true underlying value of θ used to define the data generating distribution. An estimator is unbiased if $\text{bias}(\hat{\theta}_m) = 0$, and is asymptotically unbiased if $\lim_{m \to \infty} \text{bias}(\hat{\theta}_m) = 0$. ◄

1.3.3 MAP (maximize a posteriori) estimation

Beside the MLE, one can estimate the parameters by MAP

$$\begin{aligned}
\hat{\theta}_{\text{MAP}} &= \arg\max_{\theta} p(\theta|\mathcal{D}) \\
&= \arg\max_{\theta} p(\mathcal{D}|\theta) p(\theta) \\
&= \arg\max_{\theta} \log p(\mathcal{D}|\theta) + \log p(\theta)
\end{aligned}$$

when given evidence or data $\mathcal{D}$. If we use the uniform prior $p(\theta) \propto 1$, then it reduces to a MLE.

2 Statistical Learning

In this section, we will introduce several methods in statistical learning, namely regression, classification, dimension reduction, and clustering. The first two belong to *supervised* learning, while the later two are *unsupervised*. We shall start with linear regression, which is just simple straight line fitting, to familiarize with the terminologies, as well as the optimization methods to train the regression model.

2.1 Linear regression

Ref: [CS229]

▷ Hypothesis function $h_\theta(x)$ on features x_i. For example, a multi-linear function $h_\theta(x) = \theta^T x$, where $\theta = (\theta_0, \theta_1, \ldots, \theta_n)$ are the training parameters, and $x = (1, x_1, \ldots, x_n)$ are the features.

The task is to *train* (or learn) a *model* (or hypothesis function) $h_\theta(x)$, provided the *training data* $\{(x^{(i)}, y^{(i)}), i = 1, \ldots\}$ are given. If we are then given test features x_{test}, we can make a prediction $h_\theta(x_{\text{test}})$, where θ's are the parameters trained by the training data.

▷ Cost function $J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$. The problem is to perform

$$\min_\theta J(\theta)$$

in order to minimize the *least square error*.

2.2 Training by minimization of cost function

▷ Gradient descent method: Repeat

$$\theta_j \leftarrow \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta) \quad \text{for all } j$$

until convergence. Here α is the *learning rate*.
Practical tricks: (1) feature scaling, (2) plotting $\min_\theta J(\theta)$ against number of iteractions, to ensure convergence, (3) To choose an appropriate α with the trial sequence

$$\ldots, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, 3, \ldots$$

▷ *Advanced* optimization algorithms: (1) conjugate gradient, (2) BFGS, (3) L-BFGS, (4) ADAM. These are all implemented in machine learning framework like TensorFlow. As practitioner, we may just apply the algorithms.

2.3 Regularization

If we have too few features, the learned model may be *underfitting*. If we have too many features, the learned hypothesis may fit the training set very well (overfitting) such that the training error $J(\theta) \approx 0$, but fail to generalize to new samples (make good predictions on new samples). Options: (1) reduce number of features: (i) manually select which features to keep, (ii) model selection algorithm; (2) regularization: keep all the features, but reduce magnitudes/values of parameters θ_j. This method works well when we have a lot of features, each of which contributes a bit to predicting y. This is particularly useful for NN.
Modified cost function with *regularization parameter* λ

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

The λ-term is to penalize the appearance of unnecessary features, and more importantly it controls the trade-off between the training θ in the first term and keeping θ "reasonable". (It is a convention not to include θ_0 in the regularization term, since it only shifts the fitting function $h_\theta(x)$.)
The gradient descent equation for regularized cost function suppresses θ_j in each iteration: $\theta_j \leftarrow (1 - \alpha\lambda/m)\theta_j + \cdots$ to control the overfitting problem.

2.4 Logistic regression

Also know as binary classification with two outcomes $y^{(i)} \in \{0, 1\}$. It is useful to restrict the hypothesis function $0 \le h_\theta(x) \le 1$, which serves as a *probability density function*.
▷ For linear logistic regression, the hypothesis $h_\theta(x) = P(y = 1|x; \theta)$ is

$$h_\theta(x) = g(\theta^T x)$$
$$g(z) = \frac{1}{1 + e^{-z}}$$

where $g(z)$ is the *sigmoid function* (or *logistic function*). In this case, $\theta^T x$ is the *decision boundary*.

▷ Note that the navie choice of cost function (for a particular data) $\text{Cost}\left(h_\theta(x), y\right) = \frac{1}{2}\left(h_\theta(x) - y\right)^2$, this cost function is non-convex (multiple local minima). We want the cost function for logistic regression to be convex [intuitively, Hessian matrix $H_{ij} = \partial^2 f / \partial x_i \partial x_j > 0$]. The choice is

$$\text{Cost}\left(h_\theta(x), y\right) = J(\theta) = -y \log h_\theta(x) - (1-y) \log\left(1 - h_\theta(x)\right)$$

Gradient descent formula is $\theta_j \leftarrow \theta_j - \alpha \sum_{i=1}^m \left(h_\theta(x^{(i)}) - y^{(i)}\right) x_j^{(i)}$, which is identical to linear regression.
▷ There exists a very similar approach called *support vector machines* (SVM) for binary classification tasks. One advantage of SVM is that the *kernel trick* can be applied. In this case, the decision boundary can be nonlinear. Here we shall not go into the details of SVM since it is now replaced by more general neural network approach[1]. Interested readers can consult [Goodfellow] Section 5.7.2, or [CS229] Lecture 6.

2.5 Multinomial logistic regression

Also known as *softmax regression*, or multi-category classification.
A generalization of logistic regression to the case where there are multiple classes. Here $y^{(i)} \in \{1, \dots, K\}$, where K is the number of classes. Our aim is to estimate the probability that $P(y = k|x)$ for each value of $k \in \{1, \dots, K\}$. Thus our hypothesis will output a K-dim vector, whose elements sum to 1, giving us our K estimated probabilities. Concretely, the hypothesis takes the form

$$h_\theta(x) = \begin{bmatrix} P(y=1|x;\theta) \\ P(y=2|x;\theta) \\ \vdots \\ P(y=K|x;\theta) \end{bmatrix} = \frac{1}{\sum_{k=1}^K \exp \theta^{(k)T} x} \begin{bmatrix} \exp \theta^{(1)T} x \\ \exp \theta^{(2)T} x \\ \vdots \\ \exp \theta^{(K)T} x \end{bmatrix} \equiv \text{softmax}(x; \theta^{(i)})$$

where $\theta^{(i)}$ are the training parameters for the decision boundaries of the i-th class. The cost function is

$$J(\theta) = -\left[\sum_{i=1}^m \sum_{k=1}^K \mathbb{I}(y^{(i)} = k) \log \frac{\exp \theta^{(k)T} x^{(i)}}{\sum_{k=1}^K \exp \theta^{(k)T} x^{(i)}}\right]$$

which is a negative log likeklihood (NLL), see [Murphy] Sect 8.3.7. Here $\mathbb{I}(\text{condtition}) = 1$ if condition is true, and $= 0$ otherwise.

2.6 EM for Mixture Models

Ref: [Murphy] Ch. 11
In this section, we will discuss, EM (expectation maximization) and its variant K-means algorithm, which can be used for *clustering*.
The simplest form of LVM (latent variable model) is when the latent variables $z_i \in \{1, \dots, K\}$ represents a discrete latent state. We use a discrete prior $p(z_i) = \text{Cat}(\pi)$, where π_i is the probability for each class $z_i = k$ satisfying $\pi_k \in [0, 1]$ and $\sum_k \pi_k = 1$.

► *Aside* (categorical or multinoulli distribution):

$$\text{Cat}(x|\theta) = \prod_{j=1}^K \theta_j^{\mathbb{I}(x_j = 1)}$$

◄

For the likelihood, we use $p(x_i|z_i = k) = p_k(x_i)$, where p_k is the k-th base distribution for the observations. The overall model is a mixture model for K base distributions,

$$p(x_i|\theta) = \sum_{k=1}^K \pi_k p_k(x_i|\theta)$$

[1] Though the use of kernels improves the representation power of the decision boundary, but it still cannot represent all possible functions. In the NN approach, the decision boundary is represented by the universal approximator – the NN, hence more general.

2.6.1 Issue: non-convex MAP estimate

Consider the log-likelihood for an LVM:

$$\log p(\mathcal{D}|\theta) = \sum\nolimits_i \log \left[\sum\nolimits_{z_i} p(x_i, z_i|\theta) \right]$$

The sum over z_i is inside the log function since they are hidden variables.
Suppose we consider exponential family as the joint probability distribution $p(x_i, z_i|\theta)$, then

$$p(x_i, z_i|\theta) = \frac{1}{Z(\theta)} \exp\left[\theta^T \phi(x, z)\right]$$

For complete data, the problem is easily solved. But for latent variables, the **observed data log likelihood** is

$$\ell(\theta) = \sum\nolimits_i \log \sum\nolimits_{z_i} p(x_i, z_i|\theta) = \sum\nolimits_i \log \left[\sum\nolimits_{z_i} e^{\theta^T \phi(x_i, z_i)} \right] - N \log Z(\theta)$$

One can show that the log-sum-exp function is convex, and we know that $Z(\theta)$ is convex. However, the difference of two convex functions is not, in general convex. $\implies$ Complications when applying optimization algorithms for MLE or MAP would likely face the issue of local maxima. Here the solution is provided by the EM (expectation maximization) algorithm to iteratively optimize the mixture model.

2.6.2 Basic idea

The goal is to maximize the log-likelihood of the observed data

$$\ell(\theta) = \sum\nolimits_i \log p(x_i|\theta) = \sum\nolimits_i \log \sum\nolimits_{z_i} p(x_i, z_i|\theta)$$

EM gets around the issue as follows. Define the **complete data log likelihood**,

$$\ell_c(\theta) = \sum_{i=1}^{N} \log p(x_i, z_i|\theta)$$

and the **expected complete data log likelihood** or **auxiliary function**,

$$Q(\theta, \theta^{(t-1)}) = \mathbb{E}[\ell_c(\theta)|\mathcal{D}, \theta^{(t-1)}]$$

where t is the current iteration number. The expectation is taken w.r.t the old parameters $\theta^{(t-1)}$ and the observed data $\mathcal{D}$. The **E step** is to compute the auxiliary function or the terms inside of it. In the **M step**, we optimize $Q(\theta, \theta^{(t-1)})$ w.r.t θ, namely

$$\begin{aligned} \text{MLE} \quad & \theta^{(t)} = \arg\max_\theta Q(\theta, \theta^{(t-1)}) \\ \text{MAP} \quad & \theta^{(t)} = \arg\max_\theta Q(\theta, \theta^{(t-1)}) + \log p(\theta) \end{aligned}$$

2.6.3 Variational basis for EM

Ref: [Murphy] Section 11.4.7.
It can be shown that the observed data log likelihood respects the following relation

$$\ell(\theta^{(t+1)}) \geq Q(\theta^{(t+1)}, \theta^{(t)}) \geq Q(\theta^{(t)}, \theta^{(t)}) = \ell(\theta^{(t)})$$

Hence we conclude that the EM algorithm monotonically increases the auxiliary function until it reaches a local optimum.

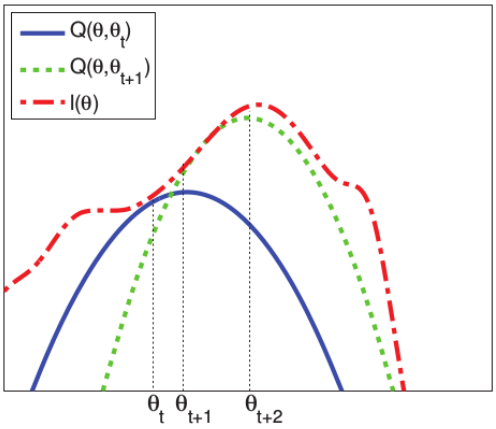


Figure 2: Illustration of EM algorithm. The parameter $\theta^{(t)}$ gives an auxiliary function $Q(\theta, \theta^{(t)})$ (E step), which is a lower bound of $\ell(\theta)$. Then we optimize $Q(\theta, \theta^{(t)})$ to give $\theta^{(t+1)}$ (M step), and then obtain the next auxiliary function $Q(\theta, \theta^{(t+1)})$. This alternating process of EM is continued until a local optimal is reached.

2.6.4 Mixtures of Gaussians

Multivariate Gaussian with mean μ_k and covariance matrix Σ_k:

$$p(x_i|\theta) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)$$

where the model parameters θ are π_k, μ_k, Σ_k. The auxiliary function is

$$\begin{aligned} Q(\theta, \theta^{(t-1)}) &= \sum_i \mathbb{E}\left[\log \prod_{k=1}^{K} [\pi_k p(x_i|\theta_k)]^{\mathbb{I}(z_i=1)}\right] \\ &= \sum_{ik} \mathbb{E}[\mathbb{I}(z_i = 1)] \log [\pi_k p(x_i|\theta_k)] \\ &= \sum_{ik} \underbrace{p(z_i = k|x_i, \theta^{(t-1)})}_{\equiv r_{ik}} \log [\pi_k p(x_i|\theta_k)] \end{aligned}$$

where r_{ik} is the **responsibility** that cluster k takes for data point i.
E step:

$$r_{ik} = \frac{\pi_k p(x_i, \theta_k^{(t-1)})}{\sum_{k'} \pi_{k'} p(x_i, \theta_{k'}^{(t-1)})}$$

M step: Optimize Q w.r.t π and θ_k. For π, we have

$$\pi_k = \frac{1}{N} \sum_i r_{ik} \equiv \frac{r_k}{N}$$

where r_k is the weighted number of points assigned to cluster k. See eqs (11.31)-(11.32) for optimized μ_k and Σ_k. After computing the new estimates, we set $\theta^{(t)} \leftarrow (\pi_k, \mu_k, \Sigma_k)$ for $k = 1, \ldots, K$ and go to the next E step.

► *Derivation for* π_k: [Murphy] Sect 3.4.3. Add a Lagrange multiplier to the auxiliary function for the constraint $\sum_k \pi_k = 1$, we need to optimize

$$\ell(\theta, \lambda) = Q(\theta, \theta^{(t-1)}) + \lambda \left(1 - \sum\nolimits_k \pi_k\right)$$

Then $\partial\ell/\partial\lambda = 0$ gives the constraint. Taking derivatives w.r.t π_k yields

$$\pi_k \propto r_k$$

and the result follows. ◀

2.7 K-means algorithm

It is a popular variant of EM for Gaussian mixture. *Simplications*: (1) the covariance matrix $\Sigma_k = \sigma^2\mathbb{I}$ is fixed, and (2) probability of classes $\pi_k = 1/K$ is fixed. Hence only the cluster centers μ_k have to be estimated. The algorithm is given below:

Algorithm 1 K-means algorithm.

1. *initialize* the cluster centers μ_k randomly
2. **repeat**
3. Assign each data point to its closet cluster center: $z_i = \arg\min_k \|x_i - \mu_k\|^2$
4. Update each cluster center by
$$\mu_k = \frac{1}{N_k}\sum_{i:z_i=k} x_i$$
5. **until** *converged*

2.8 Principal component analysis (PCA)

For dimension reduction.
Let $X = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_M \\ | & | & & | \end{bmatrix}$ be a $N \times M$ matrix, so each x_i is a N-dim column vector (data). Here M is the number of input data. We want to extract the key features in a k-dim ($k \leq N$) to represent the original N-dim data. We *assume* that the data are *centered*: $\bar{x} = \frac{1}{M}\sum_i x_i = 0$, then we can define the *covariance matrix*: $C = \frac{1}{M}\sum_i (x_i - \bar{x})(x_i - \bar{x})^T = \frac{1}{M}XX^T$. Then we solve the eigen-problem: $CU = U\Lambda$ with (orthonormal) eigenvector matrix $U = \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_N \\ | & | & & | \end{bmatrix}$ ($u_i^T u_i = 1$) and diagonal eigenvalue matrix $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$. We simply select the k largest eigenvalues and the corresponding eigenvectors as the projector $U_k = \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_k \\ | & | & & | \end{bmatrix}$. The final aim of PCA is to find the projected data y_i in the reduced k-dim: $y_i = U_k^T x_i$. It is in these (linear) projection principal vectors, the data are most spread (with the highest covariance), and hence they are the *key features*.
Inner product formulation of PCA: Notice that the eigenvectors can be expressed linearly in terms of the data $u_\alpha = \sum_i a_i^\alpha x_i$ (or symbolically $U_k = aX$), where a_i^α are yet-determined coefficients. Next, the projected data is $y_i = U_k^T x_i = (aX)^T x_i$. Note that $X^T x_i$ is an **inner product**. Hence, once we know a_i^α, we can readily perform the projection. Indeed, we can show that a_i^α are determined by the eigen-problem: $Ka = \tilde{\lambda}a$, or explicitly

$$\underbrace{(x_i^T x_j)}_{\equiv K_{ij}} a_j^\alpha = \underbrace{N\lambda_\alpha}_{\equiv\tilde{\lambda}} a^\alpha$$

where K is a $N \times N$ matrix of elements of **inner products** $x_i^T x_j$.
Notice that the resulting u_α vectors (with $\|a^\alpha\| = 1$) are not normalized, we can simply rescale $a^\alpha \to \bar{a}^\alpha$ such that $\|\bar{a}^\alpha\| = 1/\sqrt{\tilde{\lambda}_\alpha}$. Then, we obtain the projector matrix $U_k = \bar{a}X$ such that each column vector u_α is orthonormal $u_\alpha^T u_\beta = \delta_{\alpha\beta}$.

2.8.1 Kernel trick

Ref: [NeuralComputation.10.1299] "Nonlinear Component Analysis as a Kernel Eigenvalue Problem", by Schölkopf, Smola, & Müller.
In a higher dimension space, we define the mapping $\phi : X^N \to \mathcal{F}$. The input data is then $\phi(x_i)$. We want to perform PCA with the covariance matrix

$$\bar{C} = \frac{1}{M}\phi(x_i)\phi^T(x_i) = \frac{1}{M}\phi(X)\phi^T(X)$$

Naively, we can perform the mappings $\phi(x_i)$, then do PCA. But this is an inefficient method in terms of computational storage and time. We can actually find the final results, namely the projected data y_i, in a more efficient way without knowing the explicit form of ϕ and the eigenvector U by using a few *tricks*.
In the inner product formulation, the explicit knowledge of C and U is not needed, only the inner product is utilized. Hence, we simply generalize the inner product $x_i^T x_j$ in PCA to that of ϕ or the centered ψ in KPCA, namely

$$\bar{K}_{ij} = \psi^T(x_i)\psi(x_j)$$

Here $\psi(x_i) = \phi_i - \frac{1}{M}\sum_k \phi_k$ is the *centered* data after mapping ϕ, where we defined $\phi_i \equiv \phi(x_i)$. One can show that $\bar{K} = K - I_M K - K I_M + I_M K I_M$, or explicitly

$$\bar{K}_{ij} = K_{ij} - \frac{1}{M}\sum_k K_{kj} - \frac{1}{M}\sum_l K_{il} + \frac{1}{M^2}\sum_{kl} K_{kl}$$

where I_M is a $M \times M$ matrix with all elements $= \frac{1}{M}$. We need to solve the eigen-problem

$$\bar{K}\bar{a} = \tilde{\lambda}\bar{a}$$

Finally, given the new data t, the projected data after KPCA is $t' = \sum_i \bar{a}_i \bar{K}(x_i, t)$.
Kernel examples:
▷ Linear: $K(x, y) = x^T y + c$
▷ Polynomial: $K(x, y) = (ax^T y + c)^d$
▷ RBF (radial basis function) or Gaussian: $K(x, y) = e^{-\|x-y\|^2/2\sigma^2}$

3 Deep Learning

[Goodfellow] quotes: The solution for computer to learn is to allow them to learn from experience and understand the world in terms of a hierarchy of concepts, with each concept defined in terms of its relation to simpler concepts. If we draw a graph showing how these concepts are built on top of each other, the graph is deep, with many layers $\implies$ deep learning.

3.1 Universal approximation theorem

Let $\varphi(\cdot)$ be a non-constant, bounded, and monotonically-increasing continuous function. Let I_m denote the m-dimension unit hypercube $[0, 1]^m$. The space of continuous functions on I_m is denoted by $C(I_m)$. Then, given any $\varepsilon > 0$ and any function $f \in C(I_m)$, there exists an integer N, real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$, where $i = 1, \ldots, N$, such that we may define

$$F(x) = \sum_{i=1}^{N} v_i \varphi(w_i^T x + b_i)$$

as an approximate realization of the function f, where f is independent of φ; that is

$$|F(x) - f(x)| < \varepsilon$$

for all $x \in I_m$. In other words, functions of the form $F(x)$ are dense in $C(I_m)$. This still holds when replacing I_m with any compact subset of $\mathbb{R}^m$.

Ref: [Cybenko, 1989] with sigmoid activation functions
Ref: [Hornik etal., 1989] With generic activation functions, it is the multilayer feed forward architecture itself gives neural networks the potential of being universal approximators.
Ref: a visual "proof" by Michael Nelson. Basically, the function f can be discretized over I_m, and each discretized value $f(x_i)$ can be approximated by several summing step functions of various coefficients at $x_i \in I_m$.

3.1.1 Implication

In the previous section, we considered many examples of statistical learning with *linear* model $f_\theta(x) = \theta^T x$. Given the above theorem, we can replace the linear model with a NN that can represent basically any functions:

$$f_\theta(x) = \text{neural network}$$

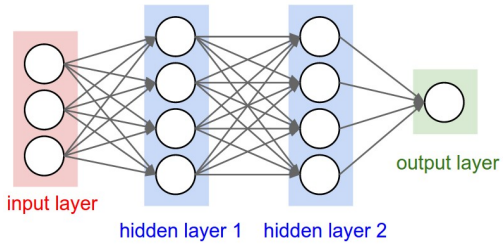
to perform the tasks of regression, classification as in statistical learning.

3.2 Neural networks

Feed-forward NN: Keywords: *input units* x, *hidden units* a.

$$x_i \to a_i^{(\ell)} \to h_\Theta(x)$$

where $a_i^{(\ell)}$ is the "activation" of unit i in layer j, and $\Theta^{(\ell)}$ is matrix of weights controlling function mapping from layer ℓ to layer $\ell + 1$



Cost function: K output nodes

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log h_\Theta(x^{(i)})_k + (1 - y_k^{(i)}) \log(1 - h_\Theta(x^{(i)})_k)\right] + \frac{\lambda}{2m}\sum_{\ell=1}^{L-1}\sum_{i=1}^{s_\ell}\sum_{j=1}^{s_{\ell+1}}(\Theta_{ij}^{(\ell)})^2$$

Forward propagation: To obtain the activation $a_j^{(\ell)}$,

$$\begin{aligned} a_i^{(\ell=1)} &= x_i \\ z_i^{(\ell)} &= \sum\nolimits_j \Theta_{ij}^{(\ell-1)} a_j^{(\ell-1)} \\ a_i^{(\ell)} &= g(z_i^{(\ell)}) \quad \text{with } g(z) = \frac{1}{1+e^{-z}} \\ h_\Theta(x)_i &\equiv a_i^{(L)} \end{aligned}$$

3.3 Back-propagation (Backprop)

BackProp is a more efficient way to obtain the gradients $\partial J(\Theta)/\partial\Theta_{ij}^{(\ell)}$ for gradient descent by computing the "error of node j in layer ℓ",

$$\begin{aligned} \delta_j^{(L)} &= a_j^{(L)} - y_j \\ \delta_i^{(\ell)} &= \sum\nolimits_j (\Theta_{ij}^{(\ell)})^T \delta_j^{(\ell+1)} \odot g'(z_i^{(\ell)}) \end{aligned}$$

Algorithm 2 Back-propagation (with regularization λ)

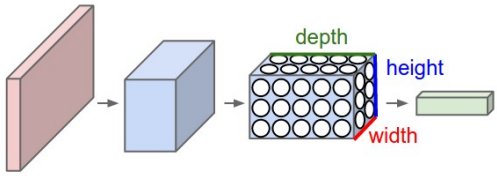
Training set $\{(x^{(i)}, y^{(i)}), i = 1, \dots, m\}$
Set $\Delta_{ij}^{(\ell)} = 0$ for all i, j, ℓ
For $i = 1$ to m {
  Set $a^{(1)} = x^{(i)}$
  Perform forward propagation to compute $a^{(\ell)}$ for $\ell = 2, 3, \dots, L$
  Using $y^{(i)}$ to compute $\delta^{(L)} = a^{(L)} - y$
  Compute $\delta^{(L-1)}, \delta^{(L-2)}, \dots, \delta^{(2)}$
  $\Delta_{ij}^{(\ell)} \leftarrow \Delta_{ij}^{(\ell)} + \delta_i^{(\ell+1)} (a_j^{(\ell)})^T$
}
$D_{ij}^{(\ell)} \leftarrow \begin{cases} \frac{1}{m}\Delta_{ij}^{(\ell)} + \lambda \Theta_{ij}^{(\ell)} & \texttt{for } j \neq 0 \\ \frac{1}{m}\Delta_{ij}^{(\ell)} & \texttt{for } j = 0 \end{cases}$

where $g'(z^{(\ell)}) = a^{(\ell)} \odot (1_{\text{v}} - a^{(\ell)})$ (1_{v} is a vector filled with 1's), and $\odot$ is the element-wise multiplication such that $(a \odot b)_i = a_i b_i$. If ignore regularization or $\lambda = 0$, then

$$\frac{\partial}{\partial \Theta_{ij}^{(\ell)}} J(\Theta) = \delta_i^{(\ell+1)} (a_j^{(\ell)})^T$$

A brief derivation is given in Appendix A.
Implementation notes: (1) unrolling parameters into vector, for better CPU optimization with vectorization; (2) gradient checking: $\partial_{\Theta_{ij}^{(\ell)}} J(\Theta) \approx [J(\Theta + \epsilon) - J(\Theta - \epsilon)]/2\epsilon$; (3) random initialization
Diagnostic: (1) Evaluating hypothesis by using random 70% of data as training set, and the rest as *test set*. Compute the test set error $J_{\text{test}}(\Theta) = \frac{1}{2m_t} \sum_{i=1}^{m_t} \left(h_\theta(x_t^{(i)}) - y_t^{(i)} \right)^2$. (2) Model selection with training set, *cross validation set*, and test set. (3) Balance between bias & variance error by plotting $J_{\text{train}}(\Theta)$ and $J_{\text{cv}}(\Theta)$ against number of features. High bias (underfit) *iff* $J_{\text{cv}}(\Theta) \sim J_{\text{train}}(\Theta)$; high variance (overfit) *iff* $J_{\text{cv}}(\Theta) \gg J_{\text{train}}(\Theta)$. (4) Learning curves against training set size m. Ref: [CS229] Lecture 7.

3.4 CNN/ConvNet



[CS231n notes]
▷ Inspired by brain experiments on visual cortex
▷ Usually used for image $\Longrightarrow$ the 1st NN layer consists of **width**, **height**, and **depth**. Here depth refers to the 3 color channels (RGB)
▷ Architecture
– `CONV`: Convolution layer. Filters are used to extract the visual features in an image. The parameters in each filter can be trained. The filters gather the *local* spatial information of a 2D image by computing a dot product between their weights and a small region they are connected to in the input volume. The number of filters become the depth of the output of this CONV layer.
Keywords: **stride**, **zero-padding** (at boundary) to maintain spatial size, useful formula $(W - F)/S + 1$
– `RELU`: element-wise activation function, such as the ReLU (rectified linear unit) $\max(0, x)$
– `POOL`: perform a downsampling operation along the spatial dimensions (width, height), such that *max pooling*.
– `NORM`: [Ioffe-Szegedy] Fallen out of favor since in practice their contribution has been shown to be minimal
– `FC`: Fully-connected layer

▷ Computational considerations: *Memory size* $\sim$ number of weights; *Computational complex* $\sim$ neuron connectivity

3.5 Recurrent NN

Ref: [colah blog] "understanding LSTM networks"

RNN: $h_t = \tanh W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$. During backprop, the weight matrix W multiplied n times, namely W^n, is needed. If the leading singular value of W is > 1 (< 1), then we have exploding (vanishing) gradient problem.

LSTM (Long short-term memory):

$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$
$$c_t = f \odot c_{t-1} + i \odot g$$
$$h_t = o \odot \tanh c_t$$

where σ is the sigmoid function, and $\odot$ denotes the element-wise product. LSTM is used to tackle the vanishing and exploding gradient problem.

Here f is the forget gate, whether to erase cell; i is the input gate, whether to write to cell; g is a gate to control how much to write to cell; and o is the output gate, how much to reveal cell. h_t and c_t are the hidden state and the cell state at time step t.

3.6 Restricted Boltzmann machines (RBM)

RBM can be used to learn a probability distribution. The NN consists of only 2 layers – visible v and hidden h. The energy in matrix notation is

$$E(v, h) = -\sum_i a^T v - b^T h - v^T W h$$

where a, b are vectors and W is a matrix, and they are the model parameters to be learned. The probability distribution has a Boltzmann form

$$P(v, h) = \frac{e^{-E(v,h)}}{Z}$$

The marginalized probability by marginalize (integrate out) the hidden layer is

$$P(v) = \frac{1}{Z} \sum_h e^{-E(v,h)}$$

4 Generative Models

– Ref: [CS231n] 2017 Lecture 13; [NIPS 2016, arxiv] Tutorial on GANs by Ian GoodFellow
– Explicit density estimation with *tractable* function: PixelCNN 2016, PixelCNN++ 2017
– Explicit density estimation with *intractable* function: Variational Autoencoder 2013
– Implicit density estimation: GANs [GAN zoo]
– Below comes from [CS229] notes2

▷ Discriminative / Generative Models: Discriminative models only try to learn $p(y|x)$, where $x \in X$ (input space) to some labels, like $y \in \{0, 1\}$ in logistic regression. Generative models also try to learn $p(x|y)$. For instance, the label $y = 1$ (dog) is given, the model would generate an image of a dog after learning a lot of examples. These probability distributions are related by the Bayes rule

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)} = \frac{p(x|y)p(y)}{\int_y p(x|y)p(y)}$$

where $p(y|x)$ is the posterior (inference, encoder), $p(x|y)$ is the likelihood (generator, decoder), and $p(y)$ is the prior.

▷ GDA (Gaussian discriminant analysis): is an *example* of generative models, given by

$$\begin{aligned} y &\sim \text{Bernoulli}(\phi) \\ x|y=0 &\sim \mathcal{N}(\mu_0, \Sigma) \\ x|y=1 &\sim \mathcal{N}(\mu_1, \Sigma) \end{aligned}$$

We can find the optimal parameters using MLE to the log-likelihood

$$\ell(\phi, \mu_0, \mu_1, \Sigma) = \sum_i \log p(x^{(i)}|y^{(i)}; \mu_0, \mu_1, \Sigma) + \sum_i p(y^{(i)}; \phi)$$

– Interestingly, if we view $p(y=1|x; \phi, \mu_0, \mu_1, \Sigma)$ as a function of x, we find that it is exactly the logistic function with θ is some appropriate function of $\phi, \mu_0, \mu_1, \Sigma$.

– GDA makes **stronger** modeling assumptions about the data than logistic regression. If these assumption are correct, then GDA will find better ftis to the data, and is a better (**asymptotically efficient**) model in the limit of large dataset. We *expect* that GDA is also more efficient for smaller dataset. In contrast, by making significantly weaker assumptions, logistic regression is more *robust* and less sensitive to incorrect modeling assumptions.

▷ Naive Bayes Classifier: Example: words x_i, and junk mail $y \in \{0, 1\}$. The likelihood is assumed to be

$$p(x_1, \dots \mid y) = \prod_i p(x_i|y)$$

5 VAE (Variational Auto-encoders)

Ref: [Kingma-Welling]. See also [blog].

– Given some dataset $\mathbf{X} = \{\mathbf{x}\}_{i=1}^N$ consisting of N i.i.d samples. We assume that the data are generated by some random process, involving an *unobserved* continuous random variable $\mathbf{z}$. The process consists of two steps: (1) a value $\mathbf{z}^{(i)}$ is generated from some prior distribution $p_{\boldsymbol{\theta}^*}(\mathbf{z})$; (2) a value $\mathbf{x}^{(i)}$ is genrate from some conditinoal distribution $p_{\boldsymbol{\theta}^*}(\mathbf{x}|\mathbf{z})$, where $\boldsymbol{\theta}^*$ is the true parameter. We assume that the prior and the likelihood come form parameteric families of distributions.

– One attempt is to use the *autoencoder*, which consists of an encoder $p_\theta(z|x)$ and a decoder $p_\theta(x|z)$, where $z \sim p_\theta(z)$. The encoder-decoder network can be trained by the ℓ_2-loss $\|x - \hat{x}\|^2$. Note that the whole AE resembles *Bayesian inference* with likelihood $p_\theta(x|z)$, prior $p(z)$, and posterior $p_\theta(z|x)$. The variational part comes from approximating the posterior $p_\theta(z|x)$ with a mean field function $q(z; \phi)$ [denoted below as $q_\phi(z|x)$].

– The **issue** is the intractability of the marginal likelihood $p_\theta(x) = \int dz p_\theta(x|z) p_\theta(z)$, as well as the posterior density $p_\theta(z|x) = p_\theta(x|z)p_\theta(z)/p_\theta(x)$, such that the EM-type algorithm cannot be applied. The **solution** given by [Kingma-Welling] is to approximate the encoder with a function $q_\phi(z|x)$.

– Firstly, we derive the variational (lower) bound for the (log) data likelihood

$$\begin{aligned} \log p_\theta(x^{(i)}) &= \mathbb{E}_{z\sim q_\phi(z|x^{(i)})}[\log p_\theta(x^{(i)})] \\ &= \mathcal{L}(\theta, \phi; x^{(i)}) + \mathbb{KL}\left(q_\phi(z|x^{(i)}) \middle\| p_\theta(z|x^{(i)})\right) \\ &\geq \mathcal{L}(\theta, \phi; x^{(i)}) \\ \mathcal{L}(\theta, \phi; x^{(i)}) &\equiv \mathbb{E}_z[\log p_\theta(x^{(i)}|z)] - \mathbb{KL}\left(q_\phi(z|x^{(i)}) \middle\| p_\theta(z)\right) \end{aligned}$$

The first line holds since $p_\theta(x^{(i)})$ does not depend on z. Then the problem becomes

$$\begin{aligned} \theta^*, \phi^* &= \arg\max_{\theta,\phi} \mathbb{E}_{x\sim p_\theta(x)} \mathcal{L}(\theta, \phi; x) \\ &= \arg\max_{\theta,\phi} \sum_{i=1}^N \mathcal{L}(\theta, \phi; x^{(i)}) \end{aligned}$$

Concerning $\mathcal{L}(\theta, \phi; x^{(i)})$, the first term is to improve the decoder through minimizing the reconstruction cost, whlie the second term is a regularizer to make the posterior $q_\phi(z|x^{(i)})$ close to the prior $p_\theta(z)$. Note that people usually choose Gaussian probability densities for $q_\phi(z|x) = \mathcal{N}\left(z\middle|\mu^{(i)}, (\sigma^{(i)})^2\right)$ and $p_\theta(z) = \mathcal{N}(z|0,1)$, hence the second term can be exactly solved. In [Kingma-Welling], the encoder $q_\phi(z|x)$ and the decoder $p_\theta(x|z)$ are modeled by NN.

5.1 Details on VAE

Ref: [bjlkeng blog]; [1606.05908] "Tutorial for VAE"; [1702.08658] "Deeper Understanding of VAE"
▷ Straightforward MLE: The aim is to maximize the log-likelihood, which can be shown [bjlkeng] as

$$\log P(X) = \frac{1}{N}\sum_{i=1}^{N} \log\left(\sum_{m=1}^{M} \mathcal{N}\left(x_i|g(z_m,\theta), \sigma^2 * I\right)\right)$$

where $P(X=x) = \int dz P(X=x, Z=z)$ marginalizing out Z. See also Eq (1) in [1702.08658].
– Two problems: (1) the log cannot be pushed inside the summation. This is not too severe since we are not deriving analytical expression here; we are fine as long as we can use gradient descent to learn θ, where the gradient is $\nabla_\theta \log p_\theta(x) = p_\theta(x)^{-1} E_{p(z)}[\nabla_\theta p_\theta(x|z)]$.
(2) Curse of dimensionality owing to the latent variables z_m: Here $P(X)$ is a complex distribution ([tutorial]: $\hat{X}$ is a shifted image should be considered closed to the input X, but its squared distance is larger than a slightly broken image), whlie we approximate it with a normal distribution. In order to approximate the integral properly, we have to sample over a huge number of z values, which is highly inefficient. It would be desirable to have an encoder $p(z|X=x)$ to select out which z_m are important for reconstructing $\hat{X}$.
▷ Aims: (a) Find $P(z)$; (b) Estimate the posterior distribution $Z|X=x_i$; (b) Use the posterior to maximize the likelihood $P(X|Z,\theta)$, which leads to the circular dependence problem. The solution by VAE is to assume $z \sim \mathcal{N}(0, I)$, *simultaneously* fit our posterior, generate samples from it, and maximize the log-likelihood function.
Using VB (variational Bayes), we find with an approximate posterior $Q(z|X)$

$$\log P(X) - \mathbb{KL}(Q(z|X)\|P(z|X)) = \mathbb{E}_{z\sim Q} \log P(X|z) - \mathbb{KL}(Q(z|X)\|P(z|X))$$

Instead of $\log P(X)$, we optimize the RHS over $\mathbb{E}_{X\sim D}$ (D is the data distribution), which is the ELBO.
▷ Reparametrization Trick: The problem for the optimization is that in the first term $\mathbb{E}_{z\sim Q} \log P(X|z)$, the sampling of z is not deterministic, hence it has no gradient and backprop cannot be applied. This can be solved by the reparametrization trick, and write the first term as

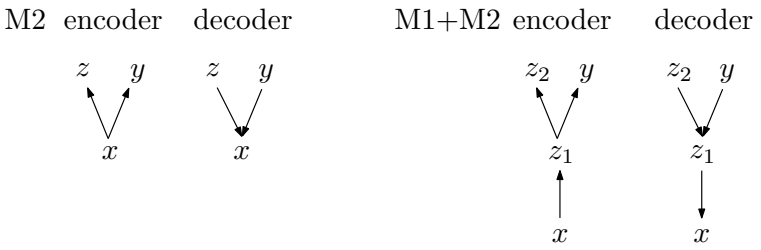
$$\mathbb{E}_{\epsilon\sim\mathcal{N}(0,I)} \log P\left(X|z = \mu_{z|X}(X;\theta) + \Sigma^{1/2}_{z|X}(X;\theta) * \epsilon\right)$$

We simply pair each observation x_i with a $\epsilon_i \sim \mathcal{N}(0, I)$, and make the loss as a deterministic function and apply the backprop.
Aside: This pairing just gives interpolation of different digits. The [VAE-SSL] paper below imposes more structures on $P(z|X)$ in order to separate the digits into different groups and correctly learn the features of the digits in each group.
▷ Interpreting the objective: [tutorial] The tractability of VAE model relies on the assumption that $Q(z|X)$ can be modeled as a normal with $\mu(X;\theta)$ and $\Sigma(X;\theta)$. $P(X)$ converges to the true distribution iff $\mathbb{KL}(Q(z|X)\|P(z|X)) \to 0$. However, it is not easy to ensure this would happen. The good news is: All we need is one decoder $g(X|z;\theta)$, which simultaneously maximizes $\log P(X)$ and results in $P(z|X)$ being normal for all X. Such decoder exists in 1D [tutorial]. See also the *information-theoretic interpretation* in [tutorial].
▷ Regularization?: It is the assumptions that $X \sim \mathcal{N}(\mu_{X|z}, \sigma^2_{X|z} * I)$ makes the first term $\mathbb{E}_{z\sim Q} \log P(X|z)$ reduces to a mean squared distance $\lambda\|X - \mu_{X|z}\|_2^2$, where $\lambda = \sigma^{-2}_{X|z}$ can be regarded as the hyperparamter for regularization. This relies on the choice of $P(X|z)$. For instance, if X is binary and we use a Bernoulli output model, then this regularization parameter disappears. See [tutorial] section 2.4.3 for more details.

5.2 VAE-Semi-Supervised Learning

[1406.5298] [bjlkeng]

▷ Basically, the VAE model add more structure to the latent code z: Given the discrete labels y, they consider several generative models



▷ Cost function:

$$\mathcal{J}^{\alpha} = \sum_{x,y\sim\tilde{p}_\ell} L(x,y) + \sum_{x\sim\tilde{p}_u} U(x) + \alpha \cdot E_{x,y\sim\tilde{p}_\ell}[-\log q_\phi(y|x)]$$

where the last term is a NLL term for the $q_\phi(y|x)$ to learn from the labeled data.

** Derive VAE-SSL eq (9): "objective (9) can also be derived directly using the variational principle by instead performing inference over the parameters π of the categorical distribution, using a symmetric Dirichlet prior over these parameters."

– Need to consider $\mathbb{KL}(q_\phi(\pi|x)\|p_\theta(\pi|y))$

– ref: [bjlkeng blog] [link] [Steck-Jaakkola-2002] "On the Dirichlet Prior & Bayesian Regularization"

5.3 Wasserstein-AE

Ref: [Wasserstein-AE]. See also [Wasserstein-GAN, zhihu].

▷ Notation: The second column shows the corresponding notation in AVE

P_X	$p_\theta(x)$	true PD (prob. density) for data X
P_Z	$p_\theta(z)$	prior for latent code Z
$P_G(X\|Z)$	$p_\theta(x\|z)$	decoder (generator)
$P_G = \int P_G(X\|Z)dP_Z$		marginal PD for X
$Q(Z\|X)$	$q_\phi(z\|x)$	approximate encoder
$Q_Z = \int Q(Z\|X)dP_X = \mathbb{E}_{P_X}[Q(Z\|X)]$		marginal PD for Z
$\mathcal{D}_Z(P_Z, Q_Z)$		regularizer for P_Z and Q_Z

▷ Generic objective function: Every AE model aims to minimize an objective function, which consists of (1) reconstruction cost, and (2) regularizer $\mathcal{D}_Z(P_Z, Q_Z)$.

▷ Issue of previous AE's: In **classical unregularized AE**, no regularizer is added. This results in different training points being encoded into non-overlapping regions chaotically scattered all across the $\mathcal{Z}$-space with "holes" in between where the decoder mapping $P_G(X|Z)$ has never been trained.

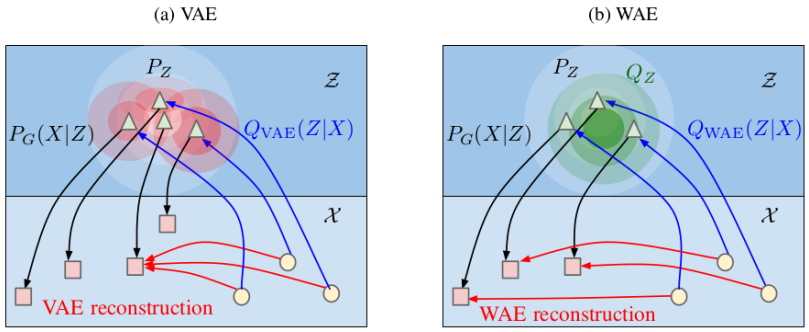


Figure 3:

In **VAE**, it forces $Q(Z|X=x)$ to match P_Z for all the different input examples x drawn from P_X. Each of these $Q(Z|X=x^{(i)})$ starts *intersecting* [see Fig 3(a)], which leads to problem with reconstruction. In contrast, WAE forces the continuous mixture $Q_Z \equiv \int Q(Z|X)dP_X$ to match P_Z. As a result latent variable z of different examples get a chance to stay away from each other, promoting a better reconstruction.
▷ In WAE, the reconstruction cost is the divergence between probability distributions induced by the optimal transport (OT)

$$W_c(P_X, P_G) \equiv \inf_{\Gamma \in \mathcal{P}(X\sim P_X, Y\sim P_G)} \mathbb{E}_{(X,Y)\sim\Gamma}[c(X,Y)]$$

where $c(x,y) : \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+$ is any measurable *cost function*, and $\mathcal{P}(X \sim P_X, Y \sim P_G)$ is a set of all *couplings* between X and Y [all joint distribution of (X,Y) with marginals P_X and P_G]. It is difficult to optimize over all couplings Γ between X and Y. The authors proves a theorem to attain the same objective by optimizing Q_Z.

► **Theorem**: For marginal distribution P_G with deterministic $P_G(X|Z)$ and any generator function $G : \mathcal{Z} \to \mathcal{X}$,

$$W_c(P_X, P_G) = \inf_{Q:\, Q_Z = P_Z} \mathbb{E}_{P_X}\mathbb{E}_{Q(Z|X)}[c(X, G(Z))]$$

where Q_Z is the marginal distribution of Z when $X \sim P_X$ and $Z \sim Q(Z|X)$. ◄

In order to relax the constraint $Q_Z = P_Z$, the authors consider the following objective function

$$D_{\text{WAE}}(P_X, P_G) = \inf_{Q(Z|X)\in\mathcal{Q}} \mathbb{E}_{P_X}\mathbb{E}_{Q(Z|X)}[c(X, G(Z))] + \lambda \cdot \mathcal{D}_Z(Q_Z, P_Z)$$

where $\mathcal{Q}$ is any non-parametric set of probabilistic encoders, $\mathcal{D}_Z$ is an arbitrary divergence between Q_Z and P_Z, and $\lambda > 0$ is a hyperparameter. Similar to VAE, the authors propose to use deep NN to parametrize both encoders Q and decoders G.
▷ They proposed 2 regularizers: (1) WAE-GAN [AAE-1511.05644], & (2) WAE-MMD (see also [1807.07306] bounded info rate-VAE; [1807.07603] doubly stochastic AAE).
▷ This work provides clear *theoretical foundation* for generic (generative) AE model.

5.3.1 Adversarial regularizer

Ref: [AAE-1511.05644]. See also [followup-VAE-WAE] folder: in particular, [slicedWAE-1804.01947] [CramerWoldAE-1805.09235]
– Recall the objection function for GAN:

$$\min_\theta \max_D L_{\text{GAN}}(D) = E_{p^*(x)} \log D(x) + E_{p_\theta(x)} \log(1 - D(x))$$

which drives $p_\theta(x)$ to learn the given probability density $p^*(x)$, due to the following fact: When $p_\theta(x)$ is fixed, the optimal $D^*(x) = \frac{p^*(x)}{p^*(x)+p_\theta(x)}$ and

$$L_{\text{GAN}}(D^*) = D_{\text{JS}}(p^*||p_\theta) + \text{const.}$$

– AAE's objective

$$\begin{aligned} E_{q_\phi(z|x)} \log p_\theta(x|z) - \mathbb{KL}[q(z)||p(z)] &= \log p_\theta(x) + I_q(x;z) - \mathbb{KL}[q(z|x)||p(z|x)] \\ &\le \log p_\theta(x) + I_q(x;z) \end{aligned}$$

Hence maximizing the objective simultaneously optimizes the NLL and the mutual info $I_q(x;z)$.

5.4 ELBO analysis

Ref: [Hoffman-Johnson-pdf] [blog]; [1702.08658] Zhao etal, "deeper understanding"; [1702.08396-VLadderAE]; [1711.00464] "Fixing a broken ELBO"; [ruishu-blog] AE a single bit

▷ [Hoffman-Johnson] There are many equivalent expressions for the VAE ELBO. Noticeably, the KL divergence term can be written as

$$\mathbb{E}_{p_{\text{data}}(x)}\mathbb{KL}(q(z|x)||p(z)) = \mathbb{KL}(q(z)||p(z)) + \mathbb{I}_{q(x,z)}(x;z)$$
$$\mathbb{I}_{q(x,z)}(x;z) = \mathbb{E}_{q(x,z)}\frac{q(x,z)}{p_{\text{data}}(x)q(z)}$$

where we defined $q(x,z) = p_{\text{data}}(x)q(z|x)$, $q(z) = \int_x q(x,z)dx$, and posterior $q(x|z) = q(z|x)p_{\text{data}}(x)/q(z)$. Hence, compared with VAE, the objective of **InfoVAE** & **AAE** is to just dropping the mutual information term $\mathbb{I}_{q(x,z)}(x;z)$ in the KL divergence term $\mathbb{KL}(q(z|x)||p(z))$. Note that maximizing VAE ELBO is to minimize $\mathbb{E}_{p_{\text{data}}(x)}\mathbb{KL}(q(z|x)||p(z))$, hence minimize the mutual information between the reconstructed data $\hat{x}$ and the latent code z. In [InfoVAE], the authors call this the **info preference problem** (or **latent variable collapse**, see below). This problem also has empirical evidence in [Bowman etal-1511.06349] & [VLossyAE-1611.02731]. In particular [VLossyAE], they observe such a problem when using a PixelCNN for the decoder. Their solution is (1) to limit the capacity of the decoder, & (2) using latent code transformed by AR flow prior, which is shown to be equivalent to using inverse AR flow (IAF) approximate posterior [IAF-1606.04934].

▷ [Zhao etal] One of the equivalent form of VAE ELBO is

$$\mathcal{L}_{\text{ELBO}} = -\mathbb{KL}(p_{\text{data}}(x)||p_\theta(x)) - \mathbb{E}_{p_{\text{data}}(x)}[\mathbb{KL}(q_\phi(z|x)||p_\theta(z|x))] \le 0$$

If the capacity of the decoder is sufficiently large (such as PixelCNN), then it is possible to attain the optimal $\mathcal{L}_{\text{ELBO}} = 0$ with $p^*(x) = p_{\text{data}}(x)$ and $p_\theta(z|x) = p(z) = q_\phi(z|x)$. In this way, the mutual information $\mathbb{I}_{q(x,z)}(x;z)$ vanishes, and leads to the info perference problem. See also [ruishu-blog]. ** *Update* [180716]: See also [1807.04863] "avoiding **latent variable collapse** with generative skip models"

In their Proposition 2, under suitable conditions, if the decoder is sufficiently large, and if the objective is only to maximize the reconstruction loss, they showed that the reconstruction loss at optimal p_{θ^*} is

$$E_{q_\phi(x,z)}[\log p_{\theta^*}(x|z)] = I_{q_\phi}(x;z) - H_{p_{\text{data}}}(x)$$

hence it is desirable to just dropping the VAE's regularizer KL term.

[VLadderAE] In particular, if the decoder has an AR (autoregressive) or Markov stacked hirarchy, then the decoder can be generated by a Gibbs chain between $\vec{z}$ and x that converges to $p_{\text{data}}(x)$ provided it is ergodic. The representation capacity of such Gibbs chain is smaller than that of the AR or Markov hirarchical decoder, and the representation capacity of the stacked architecture is wasted (low representation efficiency). They hence proposed the **VLadderAE** architecture (Fig 4), which can disentangle hirarchical feature unsupervisedly.

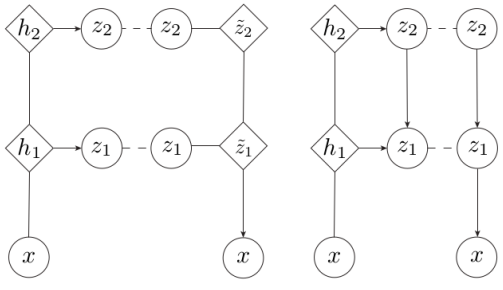


Figure 4: (Left) Variational Ladder AE; (Right) Ladder Variational AE. Key: $\rightarrow$ refers to stochastic inference; $-$ to deterministic mappings (NN); dash lines are regularization to match the prior $p(z)$. Concatenation for $\tilde{z}_\ell = u_\ell([\tilde{z}_{\ell+1}; v_\ell(z_\ell)])$, where u_ℓ, v_ℓ are NN, and $[\cdot,\cdot]$ refers to concatenation. See also [1807.04863] skip-VAE.

A significant advantage of hierarchical models for supervised learning is that they can learn rich and disentangled hierarchies of features. See [Zeiler-Fergus, 1311.2901]. However, typical HVAE (hierarchical VAE) do not enjoy this property. Suppose that $p(z|x)$ is the feature detector trained in supervised learning, and $q(z|x)$ is a approximate posterior to $p(z|x)$. It might be natural to guess that q might learn hierarchical features similar to a CNN $x \to z_1 \to \cdots \to z_L$, where higher layers correspond to higher level features that become increasingly abstract and invariant to nuisance variations.
For most models the conditional distributions $p(z_\ell|z_{>\ell})$ belong to a simple distribution family (like Gaussian). Thus for a perfectly optimized L_{ELBO} in the Gaussian case, the only type of feature hierarchy we can hope to learn is the one under which $q(z_\ell|z_{>\ell})$ is also Gaussian. (This is a result when the ELBO loss is trained to its optimal. See [HLadderAE] section 3.2 for details.) This limits the hierarchical representation we can learn. In fact, the hierarchies we observe in CNN [Zeiler-Fergus, 1311.2901] require complex multimodal distributions to be captured.

5.5 InfoVAE

Ref: [1706.02262]
Besides the info preference problem when the decoder has large capacity, if now the decoder has limited capacity, the ELBO objective would tend to sacrifice divergence in the latent code z than the reconstruction cost, resulting in bad inference. There are 2 reasons:
(i) Owing to the KL term $\mathbb{KL}(q_\phi(z|x^{(i)})||p(z))$ for each data $x^{(i)}$, the reconstruction cost can still attain large value by pushing the supports of $q_\phi(z|x^{(i)})$ and $q_\phi(z|x^{(j)})$ $(i \neq j)$ far away from each other.
(ii) Curse of dimensionality: error in $z \sim \mathcal{O}(\sqrt{n})$ implies error in $\hat{x} \sim \mathcal{O}(n)$. Hence again the reconstruction cost dominates over the regularizer term for large n (number of dimension in x).
– The problem is solved by adding by the mutual info term (see above) and combining with decoder of sufficiently large capacity.

6 Normalizing Flow

[1410.8516] NICE (Non-linear Independent Component Estimation)
[1605.08803] real NVP (real non-volume preserving)
[1807.03039] glow
[tf.distributions.bijector]
[Eric Jang blog] Modern Normalizing flows

Objective The aim is to perform a change of variable $x = g_\theta(z)$ or $z = g_\theta^{-1}(x) \equiv f(x)$ such that

$$p_X(x) = p_Z(z) \left| \det \frac{\partial z}{\partial x^T} \right|$$

▶ Consider the CDF,

$$\begin{aligned} F_X(x) &= P(X < x) = P(g(Z) < x) \\ &= P(Z < g^{-1}(x)) = F(Z < g^{-1}(x)) \end{aligned}$$

Differential both sides w.r.t. x gives

$$p_X(x) = p_Z(g^{-1}(x)) \left| \det \frac{\partial g^{-1}(x)}{\partial x} \right|$$

◀

Then given data $\{x^{(i)}\}$, one can learn the true distrubtion by MLE,

$$\min_\theta L = \mathbb{E}_{p_{\text{data}}(x)}[-\log p_X(x)] = \mathbb{E}_{p_{\text{data}}(x)} \left[-\log p_Z(f(x)) - \log \left| \det \frac{\partial f(x)}{\partial x^T} \right| \right]$$

Here we can either take $p_Z(z)$ to be some simple factorized distributions, or it can also be assumed some parametric form to be learned by MLE. The computation of the determinant can be complicated. The main objective is to design a sufficient simple form of the invertible transformation without lossing the representation power.

Affine coupling layers

▶ *Side note*: Affine transformations include identity, reflection, scaling, rotation, and shear. ◀

Forward function	Reverse function
$x_1, x_2 = \texttt{split}(x)$	$y_1, y_2 = \texttt{split}(y)$
$\log s, t = \texttt{NN}(x_2)$	$\log s, t = \texttt{NN}(y_2)$
$s = \exp(\log s)$	$s = \exp(\log s)$
$y_1 = s \odot x_1 + t$	$x_1 = (y_1 - t)/s$
$y_2 = x_2$	$x_2 = y_2$
$y = \texttt{concat}(y_1, y_2)$	$x = \texttt{concat}(x_1, x_2)$

where s and t are the **scaling** and **translation** for y_1, which are non-linear functions of the *key* x_2 represented by the NN.
Then the Jacobian of the forward function is

$$\frac{\partial y}{\partial x^T} = \begin{bmatrix} \text{diag}(s) & \frac{\partial y_1}{\partial x_2^T} \\ 0 & \mathbb{I} \end{bmatrix}$$

Multi-scale architecture (1) **Squeeze**: Transforms an $s \times s \times c$ tensor into an $\frac{s}{2} \times \frac{s}{2} \times 4c$ tensor, effectively trading spatial size for number of channels.
(2) **Flow**
(3) **Split**: factor out half of the dimensions at regular intervals such that

$$z^{(i+1)}, h^{(i+1)} = f^{(i+1)}(h^{(i)})$$

where only the intermediate "hidden" variables $h^{(i)}$ are taken to the next level of invertible transformation $f^{(i+1)}$, and the "latent" variable $z^{(i)}$ is concatenated at the last level. Note that the determinant can be composited easily: $\log|\det(dz/dx)| = \sum_i \log|\det(dh^{(i)}/dh^{(i-1)})|$

Glow (1) **Actnorm** (activation normalization): data dependent initialization $y_{i,j} = s \odot x_{i,j} + b$ where i, j are the spatial coordinates. After initialization, the scale s and bias b are treated as regular trainable parameters that are independent of the data.
(2) **Invertible** 1×1 **convolution**: As a generalization of permutation operation: $y_{i,j} = W x_{i,j}$
– *Rationale*: Notice that the coupling layers leaves part of it input unchanged, we need all the channels to influence each other. This can be done by permutation of the channels. Examing the Jacobian, we need at least 3 coupling layers. We may design some hand-coded permutations or use the 1×1 convolution to learn the permutation.
– *LU decomposition trick*: Note that the determinant Jacobian is $\propto |\det W|$ and its computation in general $\sim \mathcal{O}(c^3)$, where c is number of channels. The trick is to apply LU decomposition $W = PL(U + \text{diag}(s))$, where P, L, U are respectively permutation matrix, lower and upper triangular matrices with zeroes on the diagonal, and s is a vector. The log-determinant is simply $\log|\det W| = \texttt{sum}(\log|s|)$, scales as $\mathcal{O}(c)$.
(3) **Affine coupling layer**

7 ML in Physics

7.1 PCA – Extracting the order parameter

Ref: [PRB.94.195105] & later developments

Consider classical Ising model $H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j$. Then use MC to generate M samples for multiple number of temperatures T for a lattice of N. These date is used to construct a $M \times N$ matrices X. PCA is then performed on the data to extract the principal component. It turns out that the principal component vector (with the largest principal eigenvalue) corresponds to the order parameter in the Ising system. This result can be easily understood since it is only in this principal vector the data is "most spread" (the highest covariance) in low temperature $T < T_c$. Later development shows that the second largest principal vector corresponds to the susceptibility of the spins.
Similar methods are also applied to other physical systems but the results are not desirable due to a number of reasons: (1) For continuous symmetry breaking, enhanced flucutations of the physical degrees of freedom invalid the PCA method or its kernel variants; (2) for quantum system, the quantum fluctuations lead to similar problem. The unsupervised ML problem of order parameters seems not quite generalizable, and ML is usually used to perform phase transition detection (see below).

7.2 Classification – Phase transition detection

Ref: [nphys4035] & later developments
A NN is used to learn 2 distinct phases from MC samples. The phase transition point is determined by the maximum confusion point, that is the probability of classifying to each phase is 50%.

7.3 Regression – Acceleration for MC proposals

Ref: [PRB.95.041101] & later developments
State proposals of MC (Monte Carlo) simulations for some models can be inefficient. In this paper, they consider an effective model

$$H = \sum_i \alpha_i\tau_i + \sum_{ij}\alpha_{ij}\tau_i\tau_j + \sum_{ijk}\alpha_{ijk}\tau_i\tau_j\tau_k + \cdots$$

where τ_i are spins and α's are the parameters to be learned from the original model. This is essentially a regression problem. MC samples are first generated from the original model, then α's are fitted accordingly. Finally, only the effective model H is used to propose new states for MC simulations.

7.4 Representation power of NN – ANN for quantum many-body functions

Ref: [ncomms.8.662] "Efficient representation of quantum many-body states with RBM"
The paper proves that quantum many-body states with exponentially large Hilbert space can be *efficiently* represented by RBM (restricted Boltzmann machine) and DBM (deep Boltzmann machine) with only polynomial number of parameters. The representation power of RBM is restricted to a few classes of wavefunctions, but that of DBM is not.
Hence the Boltzmann machines can be useful for variational studies. See for instance [science.355.602], [PRB.96.205152].

7.5 Updates

– [1807.09422] Solving frustrated quantum many-particle models with CNN
— To avoid trapping in local minima, they optimize the CNN via the replica-exchange molecular dynamics method
— Minimize the total energy by SGD (stochastic gradient descent), where the energy and the gradients are calculated via MC sampling over spin configurations.

A Derivations for BackProp

Note: The derivation is **notational**. Readers should themselves fill in the details like index summations and element-wise multiplications.

Suppose the cost function is the square error function (regression)

$$J(\Theta) = \frac{1}{2}(a^{(L)} - y)^2$$

or the cross entropy (classification)

$$J(\Theta) = -y \log a^{(L)} - (1-y)\log(1-a^{(L)})$$

one can easily show that

$$\frac{\partial J}{\partial \Theta^{(L-1)}} = \delta^{(L)} a^{(L-1)}$$

where we defined

$$\delta^{(L)} = (a^{(L)} - y)$$

For the remaining layers ℓ, the **chain rule** implies

$$\begin{aligned}
\frac{\partial J}{\partial \Theta^{(\ell-1)}} &= \left(\frac{\partial J}{\partial a^{(\ell)}}\right) \frac{\partial a^{(\ell)}}{\partial z^{(\ell)}} \frac{\partial z^{(\ell)}}{\partial \Theta^{(\ell-1)}} \\
&= \left(\frac{\partial J}{\partial a^{(\ell+1)}} \frac{\partial a^{(\ell+1)}}{\partial z^{(\ell+1)}} \frac{\partial z^{(\ell+1)}}{\partial a^{(\ell)}}\right) \frac{\partial a^{(\ell)}}{\partial z^{(\ell)}} \frac{\partial z^{(\ell)}}{\partial \Theta^{(\ell-1)}} \\
&= \left(\frac{\partial J}{\partial a^{(\ell+1)}} g'(z^{(\ell+1)}) \Theta^{(\ell)}\right) g'(z^{(\ell)}) a^{(\ell-1)}
\end{aligned}$$

Note that $\frac{\partial J}{\partial \Theta^{(\ell-1)}}$ recursively depends on $\frac{\partial J}{\partial a^{(\ell)}}, \frac{\partial J}{\partial a^{(\ell+1)}}, \cdots$ of higher layers. Hence we can find $\frac{\partial J}{\partial \Theta^{(\ell-1)}}$ recursively by

$$\begin{aligned}
\frac{\partial J}{\partial \Theta^{(\ell-1)}} &= \delta^{(\ell)} a^{(\ell-1)} \\
\delta^{(\ell)} &= \Theta^{(\ell)} \delta^{(\ell+1)} g'(z^{(\ell)})
\end{aligned}$$

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