Many-body approach to the dynamics of batch learning

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Using the cavity method and diagrammatic methods, we model the dynamics of batch learning of restricted sets of examples, widely applicable to general learning cost functions, and fully taking into account the temporal correlations introduced by the recycling of the examples.

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The extraction of input-output maps from a set of examples, usually termed learning, is an important and interesting problem in information processing tasks such as classification and regression [1]. During learning, one defines an energy function in terms of a training set of examples, which is then minimized by a gradient descent process with respect to the parameters defining the input-output map. In batch learning, the same restricted set of examples is provided for each learning step. There have been attempts using statistical physics to describe the dynamics of learning with macroscopic variables. The major difficulty is that the recycling of the examples introduces temporal correlations of the parameters in the learning history. Hence previous success has been limited to Adaline learning [2], linear perceptrons learning nonlinear rules [3], Hebbian learning [4] and binary weights [5].

Recent advances in on-line learning are based on the convention of this difficulty. In contrast to batch learning, an independent example is generated for each learning step [6]. Since statistical correlations among the examples can be ignored, the dynamics can be simply described by instantaneous dynamical variables. However, on-line learning represents an ideal case in which one has access to an almost infinite training set, whereas in many applications, the collection of training examples may be costly.

In this paper, we model batch learning of restricted sets of examples, by considering the learning model as a many-body system. Each example makes a small contribution to the learning process, which can be described by linear response terms in a sea of background examples. Our theory is widely applicable to any gradient-descent learning rule which minimizes an arbitrary cost function $\{J_1\}$ of the activations $\{x_\mu\}$ and the output state $S$, $\sum_\mu g(\phi)$ as well, namely $S_\mu = f(y_\mu); y_\mu = B \cdot \xi_\mu + \phi$.

Batch learning is achieved by adjusting the weights $\{J_1\}$ iteratively so that a certain cost function in terms of the activations $\{x_\mu\}$ and the output $S_\mu$ of all examples is minimized. Hence we consider a general cost function $E = -\sum_\mu g(x_\mu, y_\mu)$. The precise functional form of $g(x, y)$ depends on the adopted learning algorithm. In previous studies, $g(x, y) = -(S-x)^2/2$ with $S = \text{sgn} x$ in Adaline learning [2], and $g(x, y) = x S$ in Hebbian learning [3].

To ensure that the perceptron is regularized after learning, it is customary to introduce a weight decay term. In the presence of noise, the gradient descent dynamics of the weights is given by

$$\frac{dJ_1(t)}{dt} = \frac{1}{N} \sum_\mu g'(x_\mu(t), y_\mu(t))\xi_\mu - \lambda J_1(t) + \eta_1(t),$$  

where the prime represents partial differentiation with respect to $x$, $\lambda$ is the weight decay strength, and $\eta_1(t)$ is the noise term at temperature $T$ with $\langle \eta_1(t) \rangle = 0$ and $\langle \eta_1(t) \rangle = 2T \delta_{jk} \delta(t-s)/N$. The dynamics of the bias $\theta$ is similar, except that no bias decay should be present according to consistency arguments [1].

$$\frac{d\theta(t)}{dt} = \frac{1}{N} \sum_\mu g'(x_\mu(t), y_\mu) + \eta_\theta(t).$$

Our theory is the dynamical version of the cavity method [6,7]. It uses a self-consistency argument to consider what happens when a new example is added to a training set. The central quantity in this method is the cavity activation, which is the activation of a new example for a perceptron trained without that example. Since the original network has no information about the new example, the cavity activation is random. Here we present the theory for $\theta = \phi = 0$, skipping extensions to biased perceptrons. Denoting the new example by the label 0, its cavity activation at time $t$ is $h_0(t) = \bar{J}(t) \cdot \xi_0$.
For large $N$, $h_0(t)$ is a Gaussian variable. Its covariance is given by the correlation function $C(t, s)$ of the weights at times $t$ and $s$, that is, $\langle h_0(t)h_0(s) \rangle = \tilde{J}(t).\tilde{J}(s) = C(t, s)$, where $\xi^p_0$ and $\xi^q_0$ are assumed to be independent for $j \neq k$. For teacher-generated examples, the distribution is further specified by the teacher-student correlation $R(t)$, given by $\langle h_0(t)y_0 \rangle = \tilde{J}(t).\tilde{B} \equiv R(t)$.

Now suppose the perceptron incorporates the new example at the batch-mode learning step at time $s$. Then the activation of this new example at a subsequent time $t > s$ will no longer be a random variable. Furthermore, the activations of the original $p$ examples at time $t$ will also be adjusted from $\{x^p_\mu(t)\}$ to $\{x^0_\mu(t)\}$ because of the newcomer, which will in turn affect the evolution of the activation of example 0, giving rise to the so-called Onsager reaction effects. This makes the dynamics complex, but fortunately for large $p \sim N$, we can assume that the adjustment from $x^p_\mu(t)$ to $x^0_\mu(t)$ is small, and linear response theory can be applied.

Suppose the weights of the original and new perceptron are $\{J_j(t)\}$ and $\{J^0_j(t)\}$ respectively. Then a perturbation of ($\ddot{1}$) yields

$$\left(\frac{d}{dt} + \lambda\right)(J^0_j(t) - J_j(t)) = \frac{1}{N}g'(x_0(t), y_0)\xi^0_j + \frac{1}{N}\sum_{\mu k} \xi^\mu_0 g''(x_\mu(t), y_\mu)\xi^k_0 (J^0_k(t) - J_k(t)).$$

(3)

The first term on the right hand side describes the primary effects of adding example 0 to the training set, and is the driving term for the difference between the two perceptrons. The second term describes the many-body reactions due to the changes of the original examples caused by the added example. The equation can be solved by the Green’s function technique, yielding

$$J^0_j(t) - J_j(t) = \sum_k \int ds G_{jk}(t, s) \left(\frac{1}{N}g'_0(s)\xi^0_k\right).$$

(4)

where $g'_0(s) = g'(x_0(s), y_0)$ and $G_{jk}(t, s)$ is the weight Green’s function, which describes how the effects of a perturbation propagates from weight $J_k$ at learning time $s$ to weight $J_j$ at a subsequent time $t$. In the present context, the perturbation comes from the gradient term of example 0, such that integrating over the history and summing over all nodes give the resultant change from $J_j(t)$ to $J^0_j(t)$.

For large $N$ the weight Green’s function can be found by the diagrammatic approach. The result is self-averaging over the distribution of examples and is diagonal, i.e. $\lim_{N \to \infty} G_{jk}(t, s) = G(t, s)\delta_{jk}$, where

$$G(t, s) = G^{(0)}(t - s) + \alpha \int dt_1 \int dt_2 G^{(0)}(t - t_1) g''_\mu(t_1)D_\mu(t_1, t_2))G(t_2, s).$$

(5)

$G^{(0)}(t - s) \equiv \Theta(t - s)\exp(-\lambda(t - s))$ is the bare Green’s function, and $\Theta$ is the step function. $D_\mu(t, s)$ is the example Green’s function given by

$$D_\mu(t, s) = \delta(t - s) + \int dt' G(t, t')g''_\mu(t')D_\mu(t', s).$$

(6)

Our approach to the macroscopic description of the learning dynamics is to relate the activation of the examples to their cavity counterparts. Multiplying both sides of ($\ddot{1}$) and summing over $j$, we get

$$x_0(t) - h_0(t) = \int ds G(t, s)g'_0(s).$$

(7)

The activation distribution is thus related to the cavity activation distribution, which is known to be Gaussian. In turn, the covariance of this Gaussian distribution is provided by the fluctuation-response relation

$$C(t, s) = \alpha \int dt' G^{(0)}(t - t')g'_\mu(t')x_\mu(s) + 2T \int dt' G^{(0)}(t - t')G(s, t').$$

(8)

Furthermore, for teacher-generated examples, its mean is related to the teacher-student correlation given by

$$R(t) = \alpha \int dt' G^{(0)}(t - t')g'_\mu(t')y_\mu.$$
the perceptron is focusing too much on the specific details of the training set. In this case $\epsilon_g$ can be optimized by early stopping, i.e., terminating the learning process before it reaches the steady state. Similar behavior is observed in linear perceptrons [4–6].

This phenomenon can be controlled by tuning the weight decay $\lambda$. The physical picture is that the perceptron with minimum $\epsilon_g$ corresponds to a point with a magnitude $|\vec{J}|$. When $\lambda$ is too strong, $|\vec{J}|$ never reaches this magnitude and $\epsilon_g$ saturates at a suboptimal value. On the other hand, when $\lambda$ is too weak, $|\vec{J}|$ grows with learning time and is able to pass near the optimal point during its learning history. Hence the weight decay $\lambda_{ot}$ for the onset of overtraining is closely related to the optimal weight decay $\lambda_{opt}$ at which the steady-state $\epsilon_g$ is minimum. Indeed, at $T = 0$ and for all values of $\alpha$, $\lambda_{ot} = \lambda_{opt} = \pi/2 - 1$: the coincidence of $\lambda_{ot}$ and $\lambda_{opt}$ is also observed previously [5]. Early stopping for $\lambda < \lambda_{ot} = \lambda_{opt}$ can speed up the learning process, but cannot outperform the optimal result at the steady state. A recent empirical observation confirms that a careful control of the weight decay may be better than early stopping in optimizing generalization [5].

At nonzero temperatures, we find the new result that $\lambda_{ot}$ and $\lambda_{opt}$ may become different. While various scenarios are possible, here we only mention the case of sufficiently large $\alpha$. As shown in the inset of Fig. 1, $\lambda_{opt}$ lies inside the region of overtraining, implying that even the best steady-state $\epsilon_g$ is outperformed by some point during its own learning history. This means the optimal $\epsilon_g$ can only be attained by tuning both the weight decay and learning time. However, at least in the present case, computational results show that the improvement is marginal.

At $T = 0$ the onset of overtraining is given by $\lambda_{ot} = \lambda_{opt}$ for random examples, whereas $\lambda_{ot} \approx \lambda_{opt}$ for teacher-generated examples. At nonzero temperatures, $\lambda_{ot}$ and $\lambda_{opt}$ become increasingly distinct, and for sufficiently large $\alpha$, $\lambda_{opt} < \lambda_{ot}$ as shown in the inset of Fig. 2, so that the optimal $\epsilon_{test}$ can only be attained by tuning both the weight decay and learning time.

3) Average dynamics: When learning has reached steady-state, the dynamical variables fluctuates about their temporal averages because of thermal noises. If we consider a perceptron constructed using the thermally averaged weights $(\bar{J}_i)_{th}$, we can then prove that it is equivalent to the perceptron obtained at $T = 0$. This equivalence implies that for perceptrons with thermal noises, the training and generalization errors can be reduced by temporal averaging down to those at $T = 0$.

We can further compute the performance improvement as a function of the duration $\tau$ of the monitoring period for thermal averaging, as confirmed by simulations in Fig. 2. Note that the Green’s function is a superposition of relaxation modes $\exp(-kt)$ whose rate $k$ lies in the range $k_{min} \leq k \leq k_{max}$, where $k_{max}$ and $k_{min}$ are $\lambda + (\sqrt{\alpha} \pm 1)^2$ respectively. For $\alpha < 1$, there is an additional relaxation mode with rate $\lambda$, which describes the relaxation by weight decay inside the $N - p$ dimensional solution space of zero training error. Hence the monitoring period scales as $k_{min}^{-1}$ for $\alpha > 1$, and $\lambda^{-1}$ for $\alpha < 1$. Note that this time scale diverges for vanishing weight decay at $\alpha < 1$. The time scale for thermal averaging agrees with the relaxation time proposed for asymptotic dynamics in [5].

We remark that the relaxation time for steady-state dynamics may not be the same as the convergence time for learning in the transient regime. For example, for $\alpha < 1$ and vanishing weight decay at $T = 0$, significant reduction of $\epsilon_t$ takes place in a time scale independent of $\lambda$, since the dynamics is dominated by a growth of the projection onto the solution space of zero training error. On the other hand, the asymptotic relaxation time diverges as $\lambda^{-1}$.
approaches the steady-state value erf(φ/√2).

Dynamics of the bias: For biased perceptrons, θ(t) approaches the steady-state value erf(φ/√2). (The failure of the student to learn the teacher bias is due to the inadequacy of Adaline rule, and will be absent in other learning rules such as back-propagation.)

The absence of bias decay modifies the dynamics of learning. For λ < √α − 1, θ(t) consists of relaxation modes with rates k in the range k\textsubscript{min} ≤ k ≤ k\textsubscript{max}, as in the evolution of the weights. Hence the weights and the bias learn at the same rate, and convergence is limited by the rate k\textsubscript{min}. However, for λ > √α − 1, θ(t) has an additional relaxation mode with rate λ = αλ/(1 + λ).

Since λ < k\textsubscript{min}, the bias learns slower than the weights, and convergence is limited by the rate λ, as illustrated in Fig. 3 which compares the evolution of the weight overlap R(t) and θ(t). If faster convergence is desired, the learning rate of the bias has to be increased.

In summary, we have introduced a general framework for modeling the dynamics of learning based on the cavity method, which is much more versatile than existing theories. It allows us to reach useful conclusions about overtraining and early stopping, input noise and temperature effects, transient and average dynamics, and the convergence of bias and weights. We consider the present work as only the beginning of a new area of study. Many interesting and challenging issues remain to be explored. For example, it is interesting to generalize the method to dynamics with discrete learning steps of finite learning rates. Furthermore, the theory can be extended to multilayer networks.

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FIG. 2. The training error at α = 0.1 and λ = 5 of the thermally averaged perceptron for random examples versus the duration τ of the monitoring period for thermal averaging. Inset: The lines of the optimal weight decay λ\textsubscript{opt} (dashed) and the onset of overtraining λ\textsubscript{opt} (solid) of the test error for teacher-generated examples at α = 3 and T = 0.3.

FIG. 3. The evolution of the teacher-student weight overlap R(t) and the bias θ(t) at α = 0.8, λ = 0.4 and T = 0.