

TTIC 31230, Fundamentals of Deep Learning

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Stochastic Gradient Descent (SGD)

The Learning Rate as Temperature

Temperature

Physical temperature is a relationship between the energy and probability.

$$P(x) = \frac{1}{Z} e^{\frac{-E(x)}{kT}} \quad Z = \sum_x e^{\frac{-E(x)}{kT}}$$

This is called the Gibbs or Boltzman distribution.

$E(x)$ is the energy of physical microstate state x .

k is Boltzman's constant.

Z is called the partition function.

Temperature

Boltzman's constant can be measured using the ideal gas law.

$$pV = NkT$$

p = pressure

V = volume

N = the number of molecules

T = temperature

k = Boltzman's constant

We can measure p , V , N and T and solve for k .

Temperature

The Gibbs distribution is typically written as

$$P(x) = \frac{1}{Z} e^{-\beta E(x)}$$

$\beta = \frac{1}{kT}$ is the (inverse) temperature parameter.

“Hot” is when β is small and “cold” is when β is large (confusing).

Temperature

In a softmax with a temperature parameter we replace energy $E(x)$ with a score $s(x)$ and drop the negative sign.

$$\text{softmax}_y[y] = \frac{1}{Z} e^{\beta s(y)}$$

We can think of the temperature parameter β as simply a parameter of this distribution.

Temperture

MCMC sampling typically involves a temperature parameter defining the distribution to be sampled from.

We do not have to worry about this now, it will be discussed in detail later.

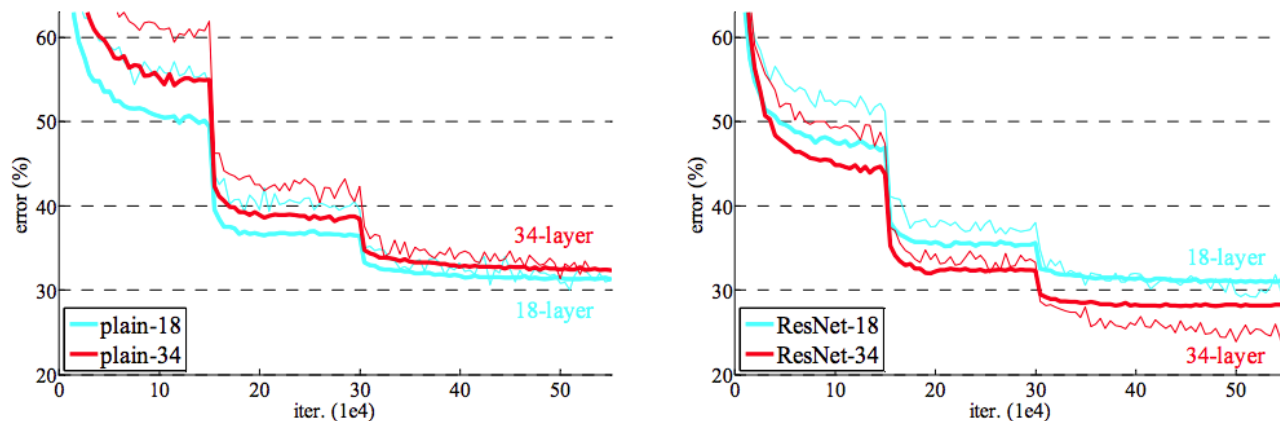
Learning Rate as Temperature

A finite learning rate defines an equilibrium probability distribution (or density) over the model parameters.

If we run for a long time at a large learning rate we converge to a noisy (hot) distribution with a high loss value.

At a lower learning rate we converge to a cooler distribution with a lower loss value.

Learning Rate as Temperature



These Plots are from the original ResNet paper. Left plot is for CNNs without residual skip connections, the right plot is ResNet.

Thin lines are training error, thick lines are validation error.

In all cases η is reduced twice, each time by a factor of 2.

Batch Size and Temperature

Vanilla SGD with minibatching typically uses the following update which defines the meaning of η .

$$\begin{aligned}\Phi_{t+1} &= \eta \hat{g}_t \\ \hat{g}_t &= \frac{1}{B} \sum_b \hat{g}_{t,b}\end{aligned}$$

Here \hat{g}_b is average gradient over the batch.

Under this update **increasing the batch size (while holding η fixed) reduces the temperature.**

Making Temperature Independent of B

For batch size 1 with learning rate η_0 we have

$$\Phi_{t+1} = \Phi_t - \eta_0 \nabla_{\Phi} \mathcal{L}(t, \Phi_t)$$

$$\begin{aligned} \Phi_{t+B} &= \Phi_t - \sum_{b=0}^{B-1} \eta_0 \nabla_{\Phi} \mathcal{L}(t+b, \Phi_{t+b-1}) \\ &\approx \Phi_t - \eta_0 \sum_b \nabla_{\Phi} \mathcal{L}(t+b, \Phi_t) \\ &= \Phi_t - B\eta_0 \hat{g}_t \end{aligned}$$

For batch updates $\Phi_{t+1} = \Phi_t - B\eta_0 \hat{g}_t$ the temperature is essentially determined by η_0 independent of B .

Making Temperature Independent of B

Recent work has show that using $\eta = B\eta_0$ leads to effective learning with very large (highly parallel) batches.

Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour, Goyal et al., 2017.

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