TTIC 31230, Fundamentals of Deep Learning

David McAllester, Autumn 2020

Stochastic Gradient Descent (SGD)

The Learning Rate as Temperature

Temperature

Physical temperature is a relationship between the energy and probability.

$$P(x) = \frac{1}{Z}\, e^{\frac{-E(x)}{kT}} \qquad Z = \sum_{x} \, e^{\frac{-E(x)}{kT}}$$

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.

$$pV = NkT$$

$$\begin{aligned} p &= \text{pressure} \\ V &= \text{volume} \\ N &= \text{the number of molecules} \\ T &= \text{temperature} \\ k &= \text{Boltzman's constant} \end{aligned}$$

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).

Loss as Energy

Learning Rate as Temperature

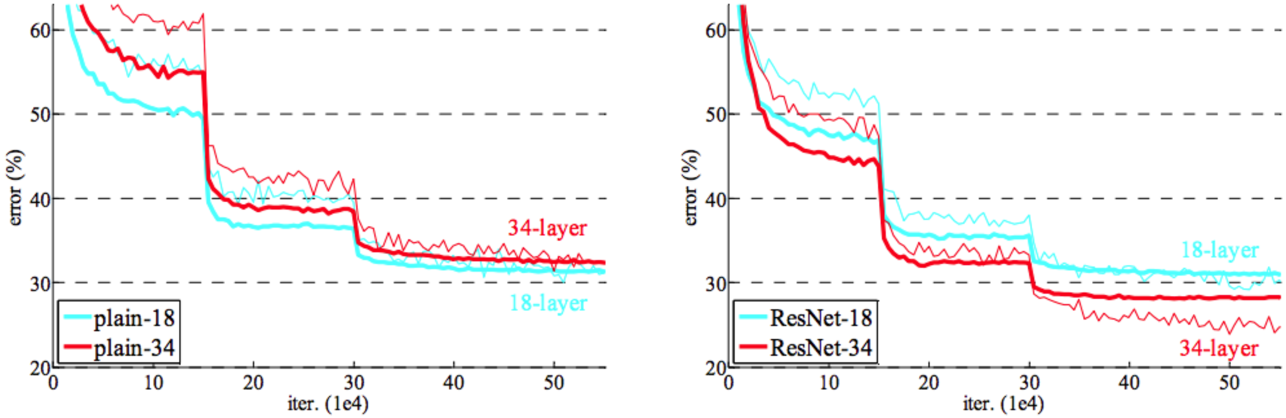
A finite learning rate defines an equalibrium probability distribution (or density) over the model parameters.

Each value of the model parameters has an associated loss.

The distribution over model parameters defines a distribution over loss.

Loss as Energy

Learning Rate as Temperature

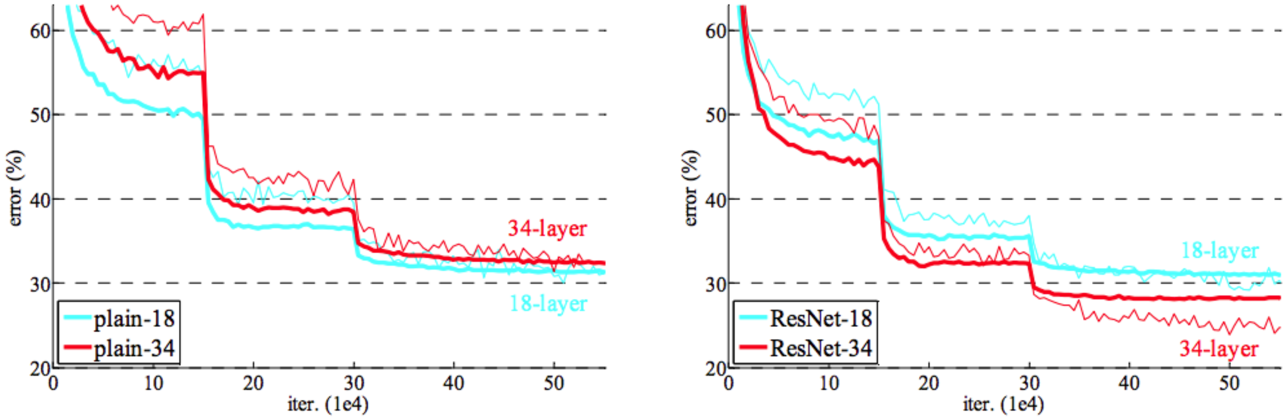


Equalibrium energy (loss) distributions at three different temperatures (learning rates).

Plots are from the 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.

Loss as Energy

Learning Rate as Temperature



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Batch Size and Temperature

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

$$\Phi_{t+1} \;\texttt{-=}\; \eta\hat{g}_t$$

$$\hat{g}_t = \frac{1}{B}\sum_b \hat{g}_{t,b}$$

Here $\hat{g}_b$ is the 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

In 2017 it was discovered that setting $\eta = B\eta_0$ allows very large (highly parallel) batches.

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

END