Geometry of Optimization and Implicit Regularization in Deep Learning

B. Neyshabur, R. Tomioka, R. Salakhutdinov, N. Srebro. 2017.

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UBC MLRG

Introduction

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  - Highly expressive
  - In general, empirical risk minimization is an NP-hard problem.

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- Consider feedforward neural networks:
    - Hypothesis class: weight vectors
    - Highly expressive
    - In general, empirical risk minimization is an NP-hard problem.
- **Why do we succeed in learning such models?**

Outline

- Implicit regularization [3]
  - Is it the network size? Or is it something else?

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  - Magnitude/scale measures for neural networks

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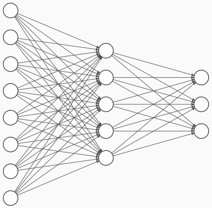
- Path-SGD [1]

Implicit Regularization

Implicit Regularization - Experiment

- D input features
- C output classes
- H hidden units, $\sigma_{\text{ReLU}}(x) = \max(0, x)$
- n training pairs



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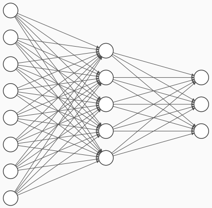

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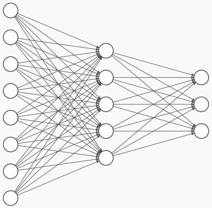
- *Truncated* softmax cross entropy loss
- SGD + momentum + diminishing step sizes
- No explicit regularization



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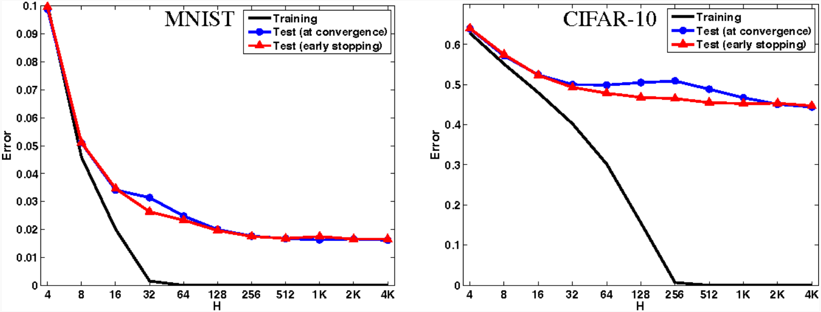
Actual results:



Implicit Regularization - Experiment

- Perhaps it's due to the optimization algorithm:
  - Tries to find a solution with small *complexity*.
  - Increasing the network size might help lower this *complexity*.

Different optimization algorithms
$\implies$ Different implicit regularization
$\implies$ Different generlization

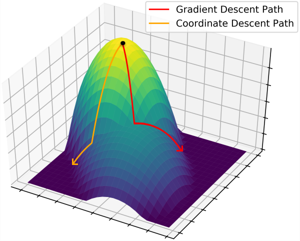


Figure 1: Gunasekar et al. https://bit.ly/32WEbXg

Geometry of Optimization

Geometry of Optimization

- Optimization is tied to a distance metric
  - Steepest descent w.r.t. ℓ_2 norm $\implies$ gradient descent
  - Steepest descent w.r.t. ℓ_1 norm $\implies$ coordinate descent
  - Steepest descent w.r.t. quadratic norm measured by the local (PD) Hessian $\implies$ Newton's method
  - Mirror descent w.r.t. entropic divergence $\implies$ exponentiated gradient descent
  - ...
- **What's the appropriate metric for neural networks?**

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- Feedforward neural network $f_{G,w,\sigma} : \mathbb{R}^D \to \mathbb{R}^C$
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- $L(w) = \frac{1}{n} \sum_{i=1}^n \ell(f_{G,w,\sigma}(x_i), y_i)$ where $\{(x_i, y_i)\}$ are training examples

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- Update step: $w^{(t+1)} = w^{(t)} + p^{(t)}$
    - For gradient descent, $p^t = -\eta^{(t)} \nabla L(w^{(t)})$

Rescaling and Unbalancedness

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  - i.e. $w^{(0)} \sim \tilde{w}^{(0)} \implies w^{(t)} \sim \tilde{w}^{(t)}$ after t updates
- We say that a network is **balanced** if the norm of the weights are roughly the same.

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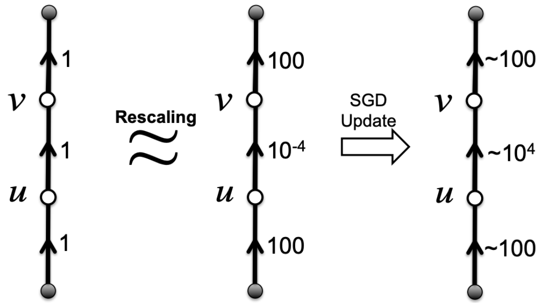
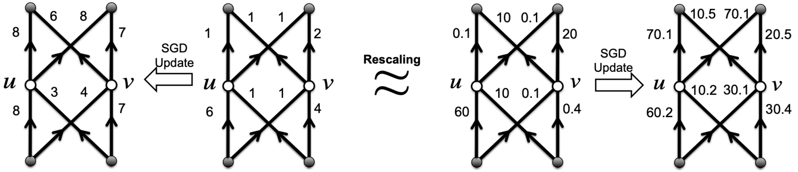
  - Scaling down the weights will scale up the gradients.
- It also performs poorly on unbalanced networks.
  - Blow up the smaller weights while keeping the larger weights almost unchanged.
- Consider $x = 1$, $\eta = 1$, $\frac{\partial L}{\partial \hat{y}} = -1$,



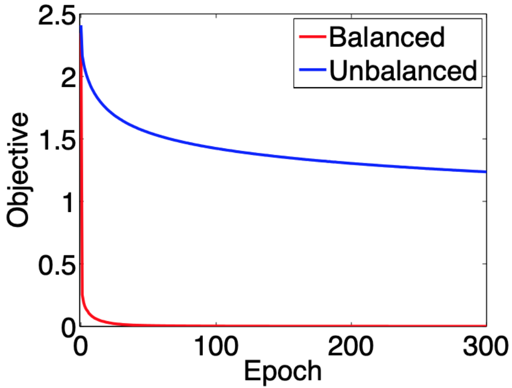
(b) Weight Explosion in an unbalanced network

Rescaling and Unbalancedness



(c) Poor updates in an unbalanced network

Rescaling and Unbalancedness



(a) Training on MNIST

Group-norm

Define the group-norm type regularizer parameterized by $p \geq 1$ and $q \leq \infty$ as,

$$\mu_{p,q}(w) = \left(\sum_{v \in V} \left(\sum_{(u \to v) \in E} \left| w_{(u \to v)} \right|^p \right)^{q/p} \right)^{1/q}$$

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- $p = q = 2$ gives us ℓ_2 regularization or weight decay.
- $p = q = 1$ gives us ℓ_1 regularization.
- $q = \infty$ gives us the per-unit "max-norm" regularization:
  - $\mu_{p,\infty}(w) = \sup_{v \in V} \left(\sum_{(u \to v) \in E} \left| w_{(u \to v)} \right|^p \right)^{1/p}$
  - Shown to be effective in ReLU networks.

Path-norm

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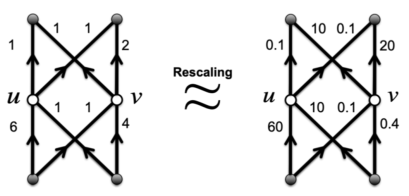

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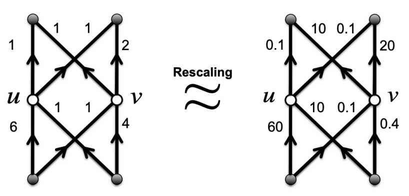

  - Left: $\mu_{1,\infty} = 7$, Right: $\mu_{1,\infty} = 70$.
- To use it as a penalty term, we should seek the minimum $\mu_{p,\infty}$ among all rescaling equivalent networks.

Path-norm

- Consider the **path vector** $\pi(w)$:
  - Number of entries $=$ number of paths from input units to output units.
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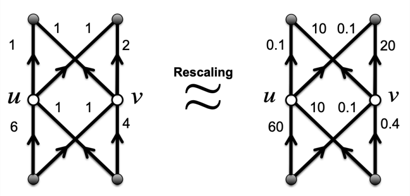
  - Number of entries = number of paths from input units to output units.
  - Each entry = product of weights along that path.
- Define the ℓ_p-**path regularizer** as

$$\|\pi(w)\|_p = \left(\sum_{v_{\text{in}}[i] \xrightarrow{e_1} v1 \xrightarrow{e_2} \dots \xrightarrow{e_d} v_{\text{out}}[j]} \left| \prod_{k=1}^{d} w_{e_k} \right|^p \right)^{1/p}.$$

Path-norm



$$\pi(w) = [6, 6, 1, 2, 1, 1, 4, 8], \qquad \|\pi(w)\|_1 = 29$$

- $\|\pi(w)\|_p$ is rescaling invariant.
- To compute it efficiently, we can use dynamic programming on the equivalent form written as nested sums.
- **Lemma [4]**: $\|\pi(w)\|_p = \min_{\tilde{w} \sim w} \left(\mu_{p,\infty}(\tilde{w})\right)^d$.

Path-SGD

Path-SGD

Steepest descent direction with respect to the path regularizer $\|\pi(w)\|_p$

$$
\begin{aligned}
w^{(t+1)} &= \arg\min_w \eta \langle \nabla L(w^{(t)}), w \rangle + \frac{1}{2} \|\pi(w) - \pi(w^{(t)})\|_p^2 \\
&= \arg\min_w \eta \langle \nabla L(w^{(t)}), w \rangle + \left(\sum_{v_{\text{in}}[i] \xrightarrow{e_1} \dots \xrightarrow{e_d} v_{\text{out}}[j]} \left(\prod_{k=1}^{d} w_{e_k} - \prod_{k=1}^{d} w_{e_k}^{(t)} \right)^p \right)^{\frac{2}{p}} \\
&= \arg\min_w J^{(t)}(w)
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\end{aligned}
$$

Update each edge weight independently,

$$
w_e^{(t+1)} = \arg\min_{w_e} J^{(t)}(w) \qquad \text{s.t. } \forall_{e' \neq e}\ w_{e'} = w_{e'}^{(t)}
$$

Path-SGD

Take the partial derivative with respect to w_e and set it to zero gives us the update rule

$$w_e^{(t+1)} = w_e^{(t)} - \frac{\eta}{\gamma_p(w^{(t)}, e)} \frac{\partial L}{\partial w}(w^{(t)})$$

where

$$\gamma_p(w, e) = \left(\sum_{v_{\text{in}}[i] \ldots \xrightarrow{e} \ldots v_{\text{out}}[j]} \prod_{e_k \neq e} |w_{e_k}|^p \right)^{2/p} .$$

Path-normalized gradient descent or **Path-SGD** when stochastic.

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Path-normalized gradient descent or **Path-SGD** when stochastic.

- Approximate steepest descent with respect to the path norm.
- Rescaling invariant.

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for $i = 1$ **to** d **do**
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end for
$\forall_{(u \to v) \in E} \ \gamma(w^{(t)}, (u, v)) = \gamma_{\text{in}}(u)^{2/p} \gamma_{\text{out}}(v)^{2/p}$
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- One update can now be computed in one forward-backward pass on a minibatch.

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- Compare ℓ_2-Path-SGD against (constant step size) SGD and AdaGrad.

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    - Both dropout ($p = 0.5$) and no dropout
    - Balanced and unbalanced initializations

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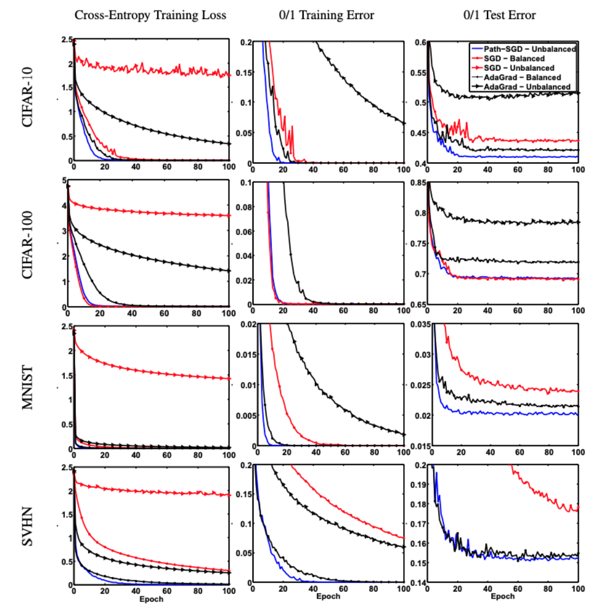
  - Both dropout ($p = 0.5$) and no dropout
  - Balanced and unbalanced initializations
- Batch size = 100

Table 1: General information on datasets used in the experiments on feedforward networks.

Data Set	Dimensionality	Classes	Training Set	Test Set
CIFAR-10	3072 (32×32 color)	10	50000	10000
CIFAR-100	3072 (32×32 color)	100	50000	10000
MNIST	784 (28×28 grayscale)	10	60000	10000
SVHN	3072 (32×32 color)	10	73257	26032

Experiment Results: without dropout



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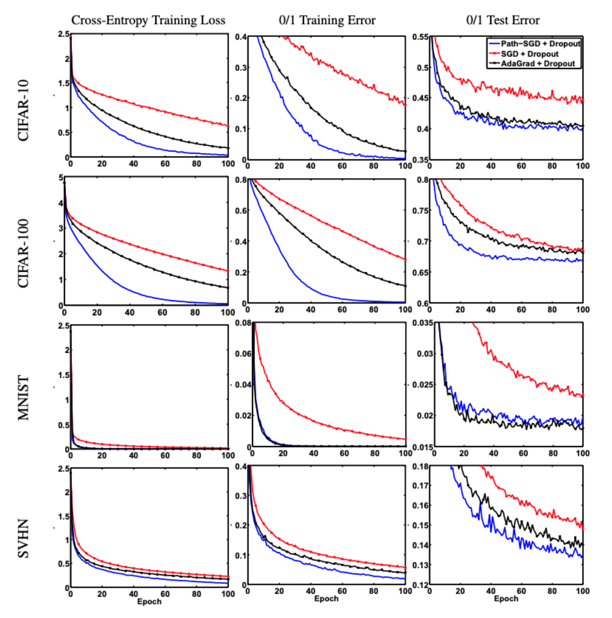

Conclusion

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Summary:

- Implicit regularization from optimization plays a role in the generalization of feedforward neural networks.
- Proposed an alternative to SGD that uses a different geomtry (path-norm) that is rescaling invariant.
- Path-SGD seems to work well compared to constant step size SGD and AdaGrad.

Conclusion

Future directions:

- Combine Path-SGD with AdaGrad?
- Other rescaling invariant metric/geometry?
- Considerations for other activation functions that don't necessarily have non-negative homogeneity?

References i

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