Nonparametric Neural Networks

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Introduction

- Problem of model selection deals with finding the best model for a given task.
- Goal of model selection: find the hyperparameter $\theta \in \Theta$ that minimizes a criterion $c(\theta)$.
- Problem: Parameter space Θ is large, thus finding optimal θ is hard.

Related Works

1. Black-box models - select a θ, test $c(\theta)$, select another θ until convergence or time over. E.g. grid search, random search, etc.
   Problem: expensive, cannot alter θ during runtime.
2. Pruning based models - Begin eliminating unnecessary weight connections from a trained model via regularization.
   Problem: require a pre-trained model to begin with.

Nonparametric Neural Networks

Optimization problem of nonparametric neural network is represented as:

$$\min_{\mathbf{d}=(d)_l, d_l \in \mathbb{Z}_+, 1 \leq l \leq L-1} \; \min_{\mathbf{W}=(w)_l, w_l \in \mathbb{R}^{d_{l-1} * d_l}, 1 \leq l \leq L} \frac{1}{|D|} \sum_{(x,y) \in D} e(f(\mathbf{W}, x), y) + \Omega(\mathbf{W})$$

d_0 and d_L are fixed because input data and error function e are fixed.
Parameters form the pair $(\mathbf{d}, \mathbf{W})$.
Fan-in and fan-out regularizers are defined as:

$$\Omega_{in}(\mathbf{W}, \lambda, p) = \lambda \sum_{l=1}^{L} \sum_{j=1}^{d_l} \|[W_l(1,j), W_l(2,j), ..., W_l(d_{l-1}, j)]\|_p$$

$$\Omega_{out}(\mathbf{W}, \lambda, p) = \lambda \sum_{l=1}^{L} \sum_{i=1}^{d_{l-1}} \|[W_l(i,1), W_l(i,2), ..., W_l(i, d_l)]\|_p$$

Outline

Controlling Network Size with Zero-Units

- Zero units are units with either fan-in or fan-out or both as zero vectors.
    - generated by fan-in or fan-out regularization.
- f-equivalence defines the notion of similarity between two network architectures $(\mathbf{d}_1, \mathbf{W}_1)$ and $(\mathbf{d}_2, \mathbf{W}_2)$: $f(\mathbf{W}_1, x) = f(\mathbf{W}_2, x)$, where not necessarily $\mathbf{d}_1 = \mathbf{d}_2$.
- Adding or removing zero-units preserves f-equivalence. (provided we use non-linearity function σ such that $\sigma(0) = 0$ - e.g. ReLu)

Outline

Self-Similar Nonlinearities

- Self-similar nonlinearities are invariant to scaling, i.e., they satisfy $\sigma(cs) = c\sigma(s), \forall c \in \mathbb{R}_{\geq 0}, s \in \mathbb{R}$ E.g. ReLu.
- Self-similar nonlinearities are required because of the usage of fan-in and fan-out regularization that shrink (or rescale) the weights.

Proposition

If all nonlinearities in a nonparametric network model except possible σ_L are self-similar, then the objective function using a fan-in or fan-out regularizer with different regularization parameters $\lambda_1, ..., \lambda_L$ for each layer is equivalent to the same objective function using the single regularization parameter $\lambda = (\prod_{l=1}^{L} \lambda_l)^{\frac{1}{L}}$ for each layer, up to rescaling of weights.

Outline

Capped Batch Normalization

- Batch normalization cannot be applied directly to nonparametric neural network as it negates the effect of regularization - since fan-in or fan-out regularizer will try to shrink the weights arbitrarily while compensating the batch normalization layer.
- Capped Batch Normalization (CapNorm) is introduced for compatibility with regularization.
- CapNorm replaces each pre-activation z with $\frac{z-\mu}{\max(\sigma,1)}$, where μ is mean and σ is standard deviation of a unit's pre-activations across the current mini-batch.

Outline

Adaptive Radial-Angular Gradient Descent (AdaRad)

input: α_r: radial step size; α_ϕ: angular step size; λ: regularization hyperparameter; β: mixing rate; ϵ: numerical stabilizer; $\mathbf{d}^0$: initial dimensions; $\mathbf{W}^0$: initial weights; ν: unit addition rate; ν_{freq}: unit addition frequency; T: number of iterations

$\phi_{\max} = 0$; $c_{\max} = 0$; $\mathbf{d} = \mathbf{d}^0$; $\mathbf{W} = \mathbf{W}^0$;

for $l = 1$ **to** L **do**

  set $\bar{\phi}_l$ (angular quadratic running average) and c_l (angular quadratic running average capacity) to zero vectors of size d_l^0;

end

for $t = 1$ **to** T **do**

  set D^t to mini-batch used at iteration t;

  $\mathbf{G} = \frac{1}{|D|}\nabla_{\mathbf{W}} \sum_{(x,y)\in D^t} e(f(\mathbf{W},x),y)$;

  for $l = L$ **to** 1 **do**

    for $j = d_l$ **to** 1 **do**

      decompose $[G_l(i,j)]_i$ into a component parallel to $[W_l(i,j)]_i$ (call it r) and a component orthogonal to $[W_l(i,j)]_i$ (call it ϕ) such that $[G_l(i,j)]_i = r + \phi$;

      $\bar{\phi}_l(j) = (1-\beta)\bar{\phi}_l(j) + \beta||\phi||_2^2$; $c_l(j) = (1-\beta)c_l(j) + \beta$;

      $\phi_{\max} = \max(\phi_{\max}, \bar{\phi}_l(j))$; $c_{\max} = \max(c_{\max}, c_l(j))$;

      $\phi_{\text{adj}} = \frac{\sqrt{\frac{\phi_{\max}}{c_{\max}}}}{\sqrt{\frac{\bar{\phi}_l(j)}{c_l(j)}} + \epsilon}\phi$;

      $[W_l(i,j)]_i = [W_l(i,j)]_i - \alpha_r r$;

      rotate $[W_l(i,j)]_i$ by angle $\alpha_\phi||\phi_{\text{adj}}||_2$ in direction $-\frac{\phi_{\text{adj}}}{||\phi_{\text{adj}}||_2}$;

      shrink$([W_l(i,j)]_i, \alpha_r\lambda\frac{|D^t|}{|D|})$;

      if $l < L$ *and* $[W_l(i,j)]_i$ *is a zero vector* **then**

        remove column j from W_l; remove row j from W_{l+1}; remove element j from $\bar{\phi}_l$ and c_l; decrement d_l;

      end

    end

    if $t = 0 \mod \nu_{freq}$ **then**

      $\nu' = \nu$;   `// if` $\nu \notin \mathbb{Z}$, `we can set e.g.` $\nu' =$ `Poisson`(ν)

      add ν' randomly initialized columns to W_l; add ν' zero rows to W_{l+1}; add ν' zero elements to $\bar{\phi}_l$ and c_l; $d_l = d_l + \nu'$;

    end

  end

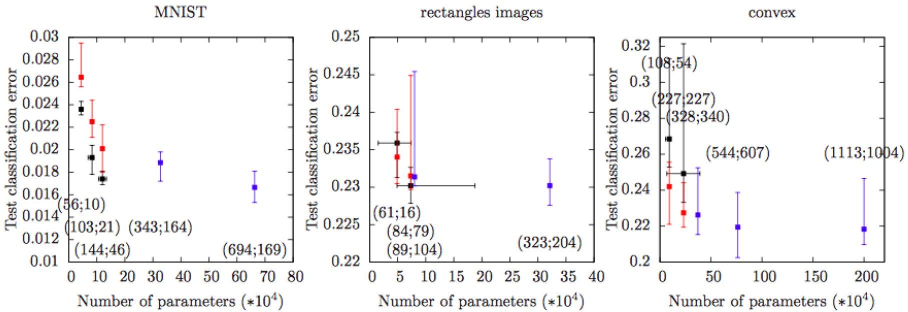
end

return $\mathbf{W}$;

Outline

Performance

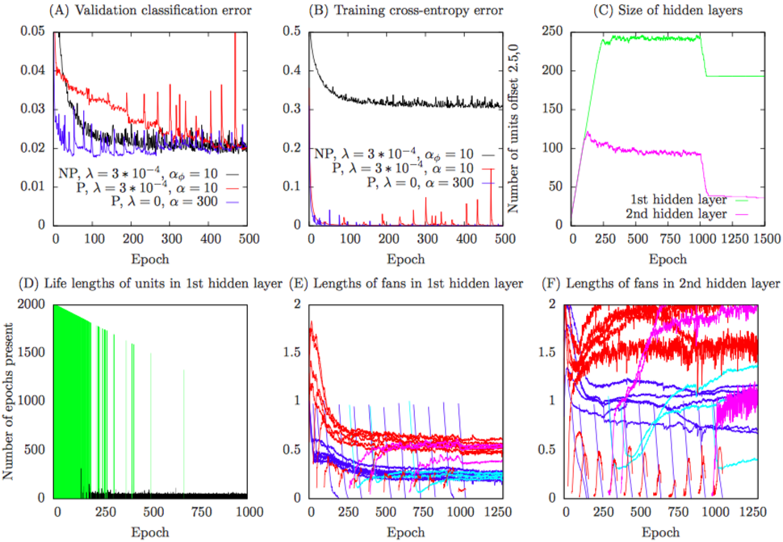
$\alpha_\phi = 30$, repeatedly divided by 3 when validation error stops improving.
$\alpha_r = \frac{1}{50\lambda}$.
λ values are $3 * 10^{-3}$, 10^{-3} and $3 * 10^{-4}$ for MNIST, $3 * 10^{-5}$ and 10^{-6} for rectangles images and 10^{-8} for convex.



Outline

Analysis of Nonparametric Training Process

$\alpha_\phi = 10$, $\lambda = 3 * 10^{-4}$. Final model has 193 X 36 units on MNIST.



Outline

Scalability

4 hidden layers instead of 2, $\alpha_r = \frac{1}{5\lambda}$, adding new units every 10th epoch.

Table 2: Test classification error of various models trained on the *poker* dataset.

Algorithm	λ	Starting net size	Final net size	Error
Logistic regression (ours)				49.9%
Naive bayes (OpenML)				48.3%
Decision tree (OpenML)				26.8%
Nonparametric net	10^{-3}	10-10-10-10	23-24-15-4	0.62%
	10^{-5}	10-10-10-10	94-135-105-35	0.022%
	10^{-6}	10-10-10-10	210-251-224-104	0.001%
	10^{-7}	10-10-10-10	299-258-259-129	0%
Parametric net		23-24-15-4	unchanged	0.20%
		94-135-105-35	unchanged	0.003%
		210-251-224-104	unchanged	0.003%
		299-258-259-129	unchanged	0.002%

Conclusion

1. Nonparametric neural network is proposed which automatically learns the optimal network structure.
2. Experimental results supporting that nonparametric neural networks outperform parametric neural networks (in most of the cases) under the same settings of network size.
3. Theoretical soundness of the framework is provided.