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UNIVERSITY LINZ

Optimal Gradient-Based Learning Using Importance Weights (Revisited)

Martin Heusel

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Institute of Bioinformatics
Johannes Kepler University, Linz, Austria

Introduction

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- Already published 2005

K. Obermayer S. Hochreiter. Optimal gradient-based learning using importance weights. In *International Joint Conference on Neural Networks (IJCNN)*, pp. 114–119, 2005.

- For difficult datasets, i.e. highly non-linear, long-term dependencies, unbalanced
- Significant speed up
- Equal or better prediction results
- Record on the “latching benchmark” sequence prediction, extract and exploit dependencies between sites which are 1,000,000 sequence elements apart

Introduction

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- How Importance Weights behave on today's large datasets, deep nets, minibatch learning, batch normalizing, dropout, multitask, multiclass, etc.?

Motivation

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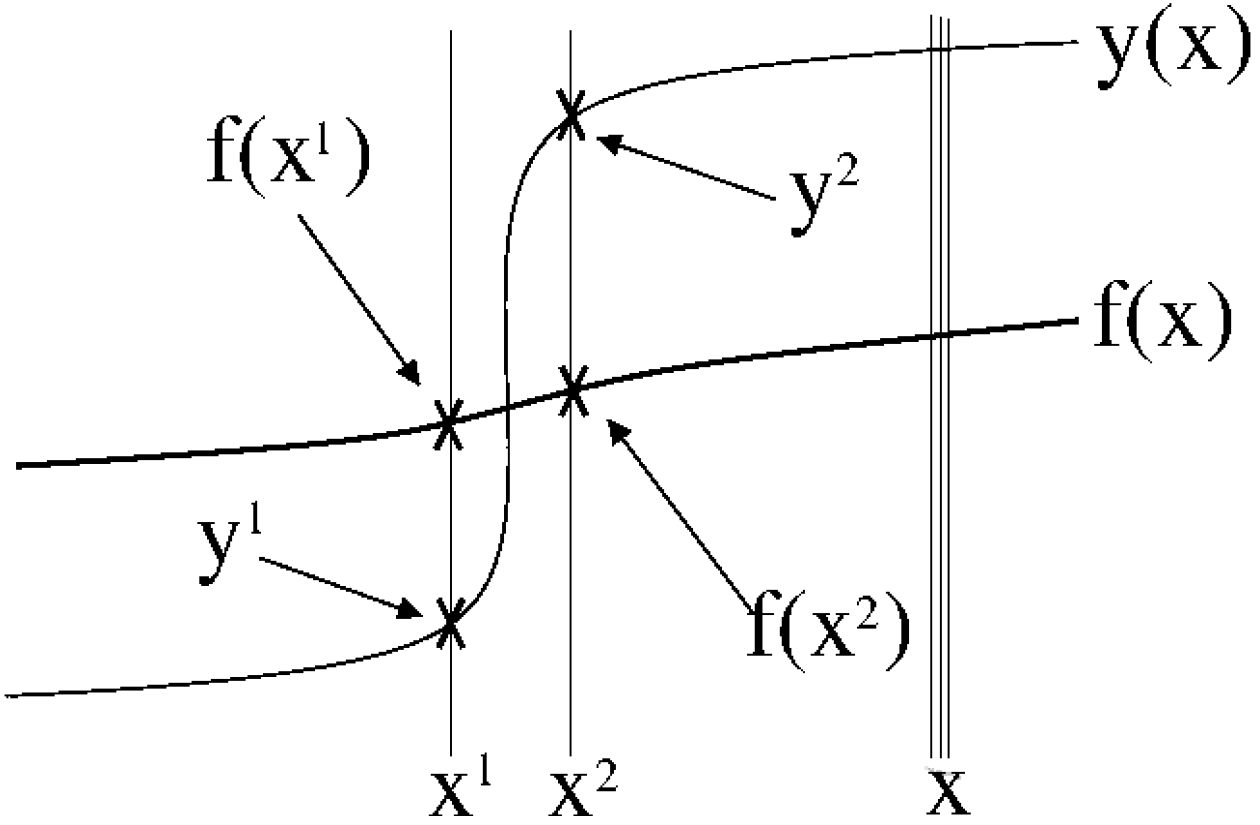

Gradient contributions at x1 and x2 cancel each other out. Gradient contributions can dominate for similar x, large classes.

Motivation

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Optimal learning step for the parameter vector **w** following two goals:

(a) The individual error for every data point decreases by at least a value of p (if possible)

(b) the associated weight change $\Delta\mathbf{w}$ should be as small a possible.

Formulation of the Optimization Problem

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Taylor expansion:

$$E(\boldsymbol{x}^i; \boldsymbol{w} + \Delta\boldsymbol{w}) \;=\; E(\boldsymbol{x}^i; \boldsymbol{w}) \;+\; \left\langle \nabla_{\boldsymbol{w}} E(\boldsymbol{x}^i; \boldsymbol{w}), \Delta\boldsymbol{w} \right\rangle \;+\; O\left(\|\Delta\boldsymbol{w}\|^2\right) \;,$$

so that decreasing the error by p leads to $\left\langle -\nabla_{\boldsymbol{w}} E(\boldsymbol{x}^i; \boldsymbol{w}), \Delta\boldsymbol{w} \right\rangle \;\geq\; p.$

Optimization problem:

$$\begin{aligned} min_{\Delta\boldsymbol{w}} \quad & \frac{1}{2}\|\Delta\boldsymbol{w}\|^2 \\ s.t. \quad & \left\langle -\nabla_{\boldsymbol{w}} E(\boldsymbol{x}^i; \boldsymbol{w}) \;,\; \Delta\boldsymbol{w} \right\rangle \;\geq\; p \end{aligned}$$

Convex Optimization Problem with Slack Variables

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- No guarantee for error improving by p for each sample i
- Slack variables ξ_i and regularization parameter C

Convex Optimization Problem with Slack Variables

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- Convex optimization problem:

$$\min_{\Delta \boldsymbol{w}} \quad \frac{1}{2}\|\Delta \boldsymbol{w}\|^2 \; + \; C \sum_i \xi_i$$

$$s.t. \quad \left\langle -\nabla_{\boldsymbol{w}} E(\boldsymbol{x}^i) \; , \; \Delta \boldsymbol{w} \right\rangle \; \geq \; p \; - \; \xi_i, \quad 0 \leq \xi_i \; .$$

- Dual formulation

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j \left\langle \nabla_{\boldsymbol{w}} E(\boldsymbol{x}^i), \nabla_{\boldsymbol{w}} E(\boldsymbol{x}^j) \right\rangle \; - \; p \; \sum_i \alpha_i$$

$$s.t. \quad 0 \leq \alpha_i \leq C \; .$$

Importance Weights

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- New learning step using Karush-Kuhn-Tucker conditions:

$$\begin{aligned} \Delta \boldsymbol{w} &= -\sum_i \alpha_i \, \nabla_{\boldsymbol{w}} E(\boldsymbol{x}^i) \quad \text{and} \\ \|\Delta \boldsymbol{w}\|^2 &= p \sum_i \alpha_i + C \sum_{i:\alpha_i = C} \xi_i \; . \end{aligned}$$

- α_i are importance weights for training vectors and individual step sizes for standard gradient update rule
- Importance weights by minimizing contributions of coupling strengths $\left\langle \nabla_{\boldsymbol{w}} E(\boldsymbol{x}^i), \nabla_{\boldsymbol{w}} E(\boldsymbol{x}^j) \right\rangle$

Fast SMO Version

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- Using old solutions for the α_i leads to faster new solutions if only a few $\alpha_i \neq 0$
- Finding α_i , α_j which yield largest update
- Choice of α and search is efficient because no equality constraint

Sparse Solution / New LOO Bound

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- $\alpha_i = 0$ for pairs of data points with similar gradient information which is common in today's large datasets
- α_i large for antiparallel gradients
- Controlled by parameters p and C
- Data points never learned, LOO almost unbiased $\rightarrow$
- New bound on generalization error using LOO estimators analog to bounds for SVMs

Experiments

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- Hemoglobin protein sequences, three species
- Protein remote homology fold prediction on SCOP data, 318 fold classes

Hemoglobin Protein Sequences

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- 736 Hemoglobin A protein sequences from the organisms Mammials, Fish and Sauria from Uniprot
- Class size ratios 384:93:259 respectively
- Randomly allocate sequences into training and test, ratio 4:1
- (j)LSTM with SGD, Adadelta and Importance Weights
- 20 Memory Cells, sliding window 5
- Learning rate fixed to 0.01, online learning
- Parameters p and C for Importance Weights fixed to 0.1 each
- Softmax, Cross-Entropy Loss

Hemoglobin Protein Sequences

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```
CLUSTAL O(1.2.1) multiple sequence alignment


fish        -SLSAKDKANVKAIWGKILPKSDEIGEQALSRMLVVYPQTKAYFSHWASVAPGSAPVKKH
bird        MVLSAADKTNVKGVFSKIGGHADDYGAETLERMFIAYPQTKTYFPHFD-LQHGSAQIKAH
human       MVLSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHFD-LSHGSAQVKGH
              **  **:***. :.*:  :: : * ::*.**:: :* **:** *:  :  *** :* *

fish        GITIMNQIDDCVGHMDDLFGFLTKLSELHATKLRVDPTNFKILAHNLIVVIAAYFPAEFT
bird        GKKVAAALVEAVNHIDDIAGALSKLSDLHAQKLRVDPVNFKFLGHCFLVVVAIHHPXALT
human       GKKVADALTNAVAHVDDMPNALSALSDLHAHKLRVDPVNFKLLSHCLLVTLAAHLPAEFT
            * .:   : :.* *:**:   *: **:*** ******.***:*.* ::*.:* : *  :*

fish        PEIHLSVDKFLQQLALALAEKYR
bird        PEVHASLDKFMCAVGAVLTAKYR
human       PAVHASLDKFLASVSTVLTSKYR
            * :* *:***:  :. .*: ***
```

Hemoglobin 3 Class Prediction
Top 1 Error

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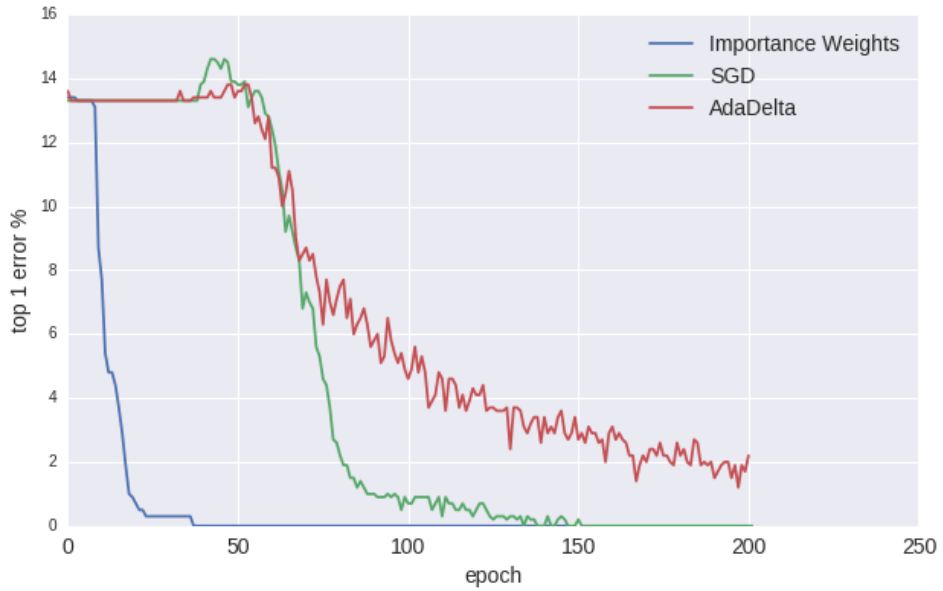
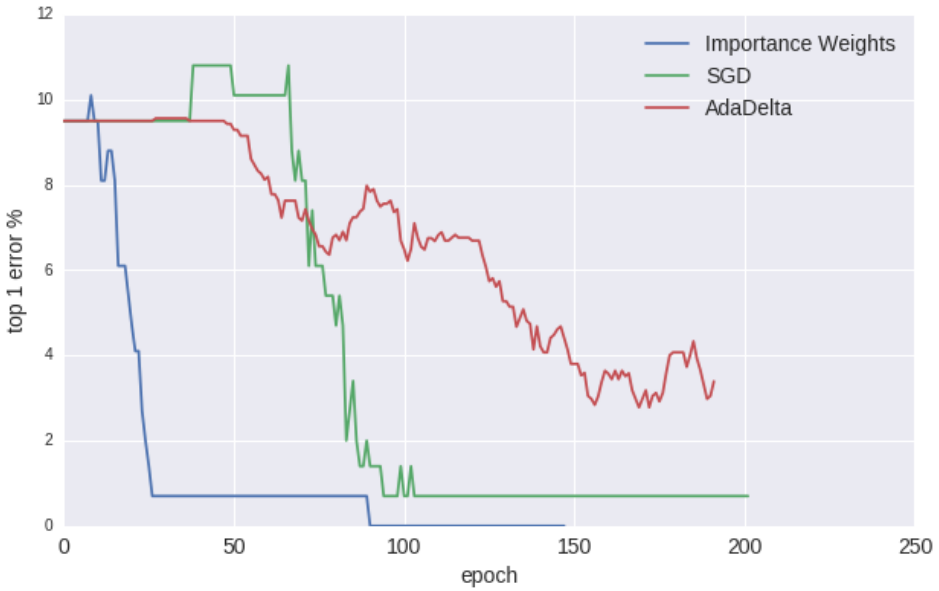


Training



Test

SCOP Protein Remote Homology Fold Prediction

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- SCOP (Structural Classification of Proteins)
- Database of experimentally measured Protein folds
- Coordinate data mostly derived from Protein Data Bank
- Tree hierarchy of class, fold, superfamily, family, sequence
- SCOP 2.06: 77439 PDB entries, 7 classes, 1221 folds, 2008 superfamilies, 4851 families

SCOP FASTA Sequences

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>d1rfya_ a.2.13.1 (A:) Transcriptional repressor TraM {Agrobacterium tumefaciens [TaxId: 358]}
KKVELRPLIGLTRGLPPTDLETITIDAIRTHRRLVEKADELFQALPETYKTGQACGGPQHIRYIEASIEMHAQMSALNTLISILGFIPK
>d1us6b_ a.2.13.1 (B:) Transcriptional repressor TraM {Agrobacterium tumefaciens [TaxId: 358]}
MELEDANVTKKVELRPLIGLTRGLPPTDLETITIDAIRTHRRLVEKADELFQALPETYKTGQACGGPQHIRYIEASIEMHAQMSALNTLYSILGFIPKVV
>d2hjda_ a.2.13.1 (A:) automated matches {Agrobacterium tumefaciens [TaxId: 358]}
FELRPVIGLTRGLSSADIETLTANAIRLHRQLLEKADQLFQVLPDDIKIGTAAGGEQHLEYIEAMIEMHAQMSAVNTLVGLLGFIPKVS
>d2qalr1 a.4.8.1 (R:19-73) Ribosomal protein S18 {Escherichia coli [TaxId: 562]}
EIDYKDIATLKNYITESGKIVPSRITGTRAKYQRQLARAIKRARYLSLLPYTDRH
>d2fnaa1 a.4.5.11 (A:284-356) Hypothetical protein SSO1545, C-terminal domain {Sulfolobus solfataricus [TaxId: 2287]}
REIARKRYLNIMRTLSKCGKWSDVKRALELEEGIEISDSEIYNYLTQLTKHSWIIKEGEKYCPSEPLISLAFS
>d2foka1 a.4.5.12 (A:5-143) Restriction endonuclease FokI, N-terminal (recognition) domain {Flavobacterium okeanokoites [TaxId: 244]}
IRTFGWVQNPGKFENLKRVVQVFDRNSKVHNEVKNIKIPTLVKESKIQKELVAIMNQHDLIYTYKELVGTGTSIRSEAPCDAIIQATIADQGNKKGYIDNW...
>d4kphl1 b.1.1.0 (L:1-107) automated matches {Mouse (Mus musculus) [TaxId: 10090]}
EIVLTQSPAIMSASLGEEITLTCSASSSVNYMHWYQQKSGTSPKLLIYTTSNLASGVPSRFSGSGSGTFYSLTISSVEAEDAADYYCHQWSSYPTFGGGTKLEIK
>d4p46a1 b.1.1.0 (A:2-111) automated matches {Mouse (Mus musculus) [TaxId: 10090]}
QVRQSPQSLTVWEGETAILNCSYENSAFDAFPWYQQFPGEGPALLIAIRSVSDKKEDGRFTIFFNKREKKLSLHITDSQPGDSATYFCAASKGADRLTFGKGTQLIIQP
>d5buva1 b.82.1.0 (A:2-173) automated matches {Yersinia enterocolitica [TaxId: 393305]}
IINITELNISGCYLIESPIFSDERGEFVKTHHQEIFKNFGLEIPSAEEYYSRSKNNVIRGMHFQQYPDDHNKLVFCPEGEVLDVFLDIRKDSNTYGQFMSFILNPHNRRSI...
>d1ep0a_ b.82.1.1 (A:) dTDP-4-dehydrorhamnose 3,5-epimerase RmlC {Methanobacterium thermoautotrophicum [TaxId: 145262]}
EFRFIKTSLDGAIIIEPEVYTDERGYFMETFNEAIFQENGLEVRFVQDNESMSVRGVLRGLHFQREKPQGKLVRVIRGEIFDVAVDLRKNSDTYGEWTGVRLSDENRREFFI...
>d2xwsa1 c.92.1.3 (A:1-125) automated matches {Archaeoglobus fulgidus [TaxId: 2234]}
MRRGLVIVGHGSQLNHYREVMELHRKRIEESGAFDEVKIAFAARKRRPMPDEAIREMNCDIIYVVPLFISYGLHVTEDLPDLLGFPRGRGIKEGEFEGKKVVICEPIGE...
>d3pdia_ c.92.2.0 (A:) automated matches {Azotobacter vinelandii [TaxId: 322710]}
GCAKPKPGATDGGCSFDGAQIALLPVADVAHIVHGPIACAGSSWDNRGTRSSGPDLYRIGMTTDLTENDVIMGRAEKRLFHAIRQAVESYSPPAVFVYNTCVPALIGD...
>d1jdqa1 d.68.3.3 (A:20-98) Hypothetical protein TM0983 {Thermotoga maritima [TaxId: 2336]}
MAKYQVTKTLDVRGEVCPVPDVETKRALQNMKPGEILEVWIDYPMSKERIPETVKKLGHEVLEIEEVGPSEWKIYIKVK
>d1j7ha_ d.79.1.1 (A:) Conserved 'hypothetical' protein YjgF {Haemophilus influenzae [TaxId: 727]}
MMTQIIHTEKAPAAIGPYVQAVDLGNLVLTSGQIPVNPATGEVPADIVAQARQSLENVKAIIEKAGLTAADIVKTTVFVKDLNDFAAVNAEYERFFKENNHPNFP...
>d4y28j_ f.23.18.0 (J:) automated matches {Pea (Pisum sativum) [TaxId: 3888]}
RDLKTYLSVAPVASTLWFAALAGLLIEINRLFPDALTFPFF
>d1jb0j_ f.23.18.1 (J:) Subunit IX of photosystem I reaction centre, PsaJ {Synechococcus elongatus [TaxId: 32046]}
MKHFLTYLSTAPVLAAIWMTITAGILIEFNRFYPDLLFHPL
>d4kt0j_ f.23.18.1 (J:) automated matches {Synechocystis sp. [TaxId: 1148]}
MDGLKSFLSTAPVMIMALLTFTAGILIEFNRFYPDLLFHP

Astral Database

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- Astral database maintains sequence similarity filtered sequences from SCOP
- 28010 sequences with max 95% similarity

Dataset construction

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- Astral 95%
- Discarded 2 classes: Multidomain proteins, small proteins
- 25943 sequences left, 318 folds
- Remote homology detection (divergent evolution)
- Superfamilies have low inter similarities
- Difficult prediction, not possible with simple alignment methods e.g. PSI-BLAST ROC 0.7 ROC50 0.26
- For each fold with > 4 superfamilies, use superfamily with median size within this fold as left out test sequences

Dataset

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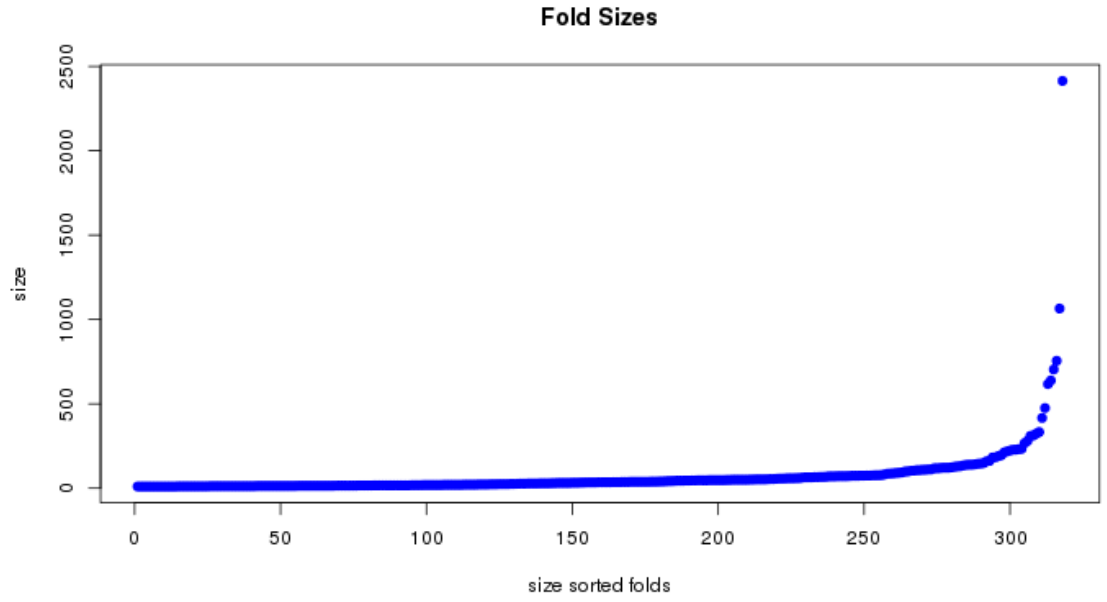
- 23435 sequences for training, 318 folds
- 184 sequences for test, 67 folds



Model

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- (j)LSTM
- 200 Memory Cells
- Sliding window size 5
- Minibatch 500
- Learning rate for SGD 0.01, 4 threads
- p 0.1, C 1.0 for Importance Weights, jOptimizer, GPU, 1 thread, p * loss
- dW cut 1.0
- no dropout, no batch normalization

SCOP Fold Prediction
Top 1/5 Error Training/Test

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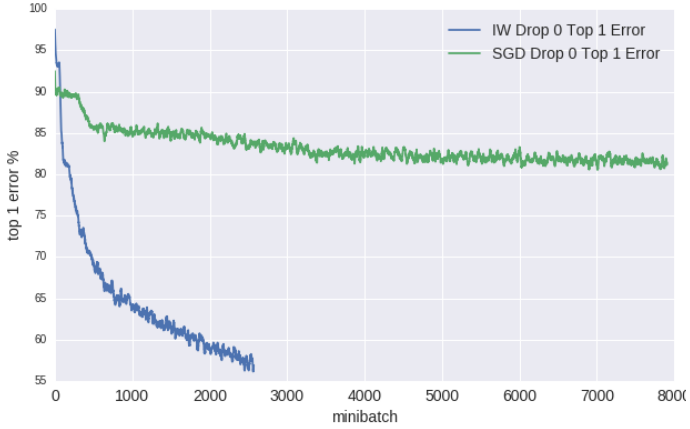
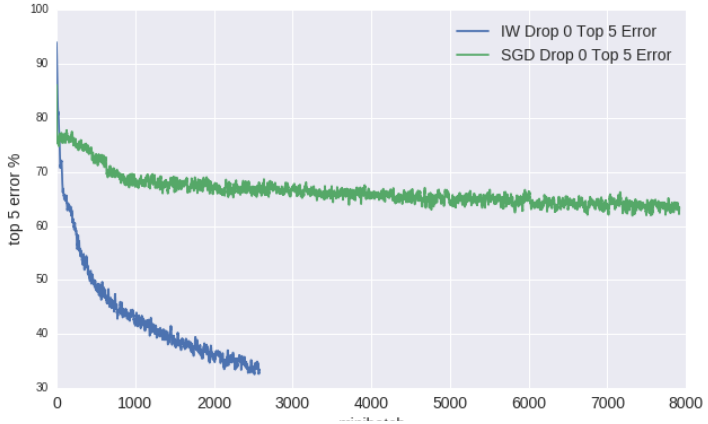
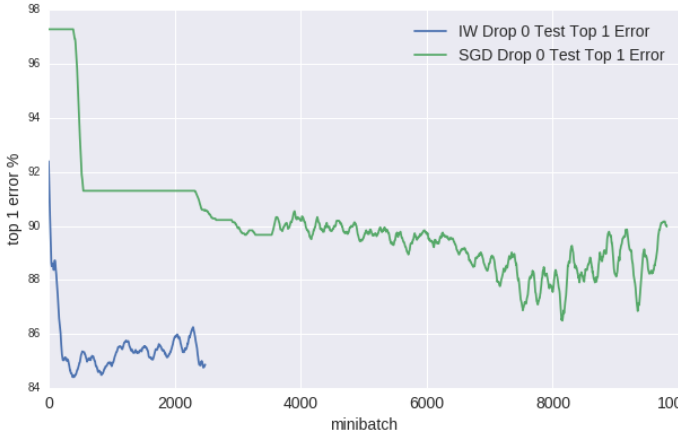
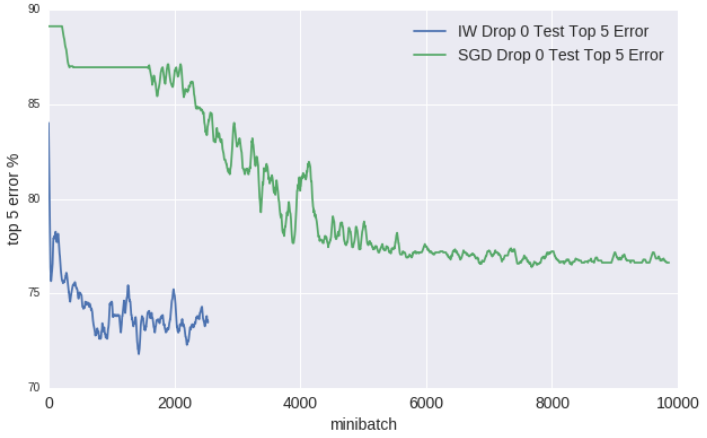
Training





Test





SCOP Fold Prediction
Cross-Entropy Loss Training/Test

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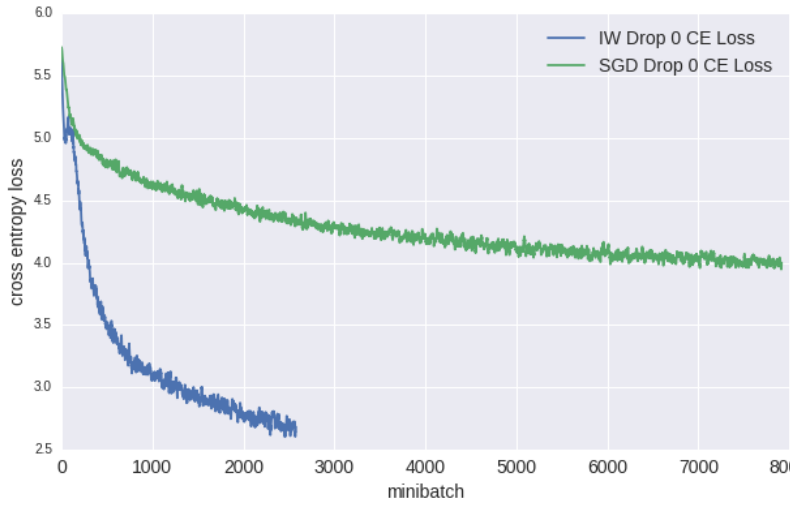
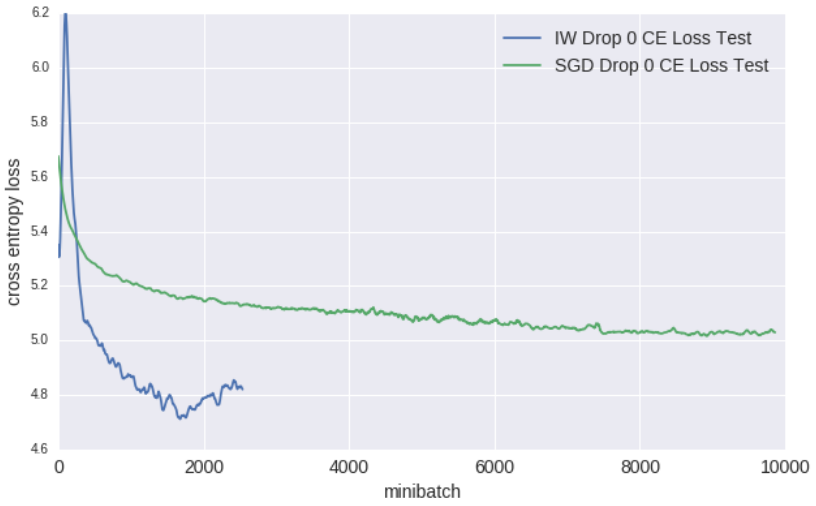


Training



Test

Class Test Accuracies Sorted By Class Size

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