# Classification

- CLS 3a. Stochastic Gradient Decent
- CLS 3b. Evaluation Metrics



1

## Risk Minimization with Training Data

$\{(x_i, y_i)\}_{i=1}^n$: training data $\overset{i.i.d.}{\sim} \mathcal{D}$.

$$\min_f \underbrace{\mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}} \ell\left(f\left(x\right), y\right)}_{\text{True risk}} \Longrightarrow \min_f \underbrace{\frac{1}{n}\sum_{i=1}^n \ell\left(f\left(x_i\right), y_i\right)}_{\text{Empirical risk}} \quad (1)$$

$$\Longrightarrow \min_w \frac{1}{n}\sum_{i=1}^n \ell\left(f_w\left(x_i\right), y_i\right) \quad (2)$$



2

# Risk Minimization with Training-set Loss Regularization

| **Classifer** | $\ell\left(f_w(x_i), y_i\right)$ | Regulurization |
|---|---|---|
| Logistic Regression | $\ln\left(1+e^{-y_i w^\top x_i}\right)$ | $\frac{\lambda}{2}\|w\|^2$ |
| SVM | $\max\left(0, 1-y_i w^\top x_i\right)$ | $\frac{\lambda}{2}\|w\|^2$ |

SVM (Support Vector Machines): typical large-margin classification model





# Gradient Descent (GD)

- Training Objective (omit regularization term for simplicity)

$$\min_w l(w) \tag{3}$$

where $l(w) \stackrel{\text{def}}{=} \frac{1}{n}\sum_{i=1}^n l_i(w) \stackrel{\text{def}}{=} \frac{1}{n}\sum_{i=1}^n l(f_w(x_i), y_i)$

- Gradient Update

$$w^{(k)} := w^{(k-1)} - \eta_k \nabla l(w^{(k-1)})$$

  - $\eta_k$ if pre-specified or determined via backtracking
  - If the loss function is not smooth, then using sub-gradient (e.g., SVM's loss is piece-wise linear).

# How fast does GD converge?

- Theorem

*If $\ell$ is both convex and differentiable* [1]

$$\ell\left(w^{(k)}\right)-\ell\left(w^{*}\right) \leq \begin{cases} \frac{\|w^{(0)}-w^{*}\|_2^2}{2\eta k} = O\left(\frac{1}{k}\right) & \ell \text{ is convex} \\ \frac{c^k L\|w^{(0)}-w^{*}\|_2^2}{2} = O\left(c^k\right) & \ell \text{ is strongly convex} \end{cases} \tag{4}$$

where k is the number of iterations and $c \in (0,1)$.

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1: the step size $\eta$ must be no larger than $\frac{1}{L}$ where $L$ is the Lipschitz constant satisfying $\|\nabla \ell(a) - \nabla \ell(b)\|_2 \leq L\|a-b\|_2 \ \forall a, b$





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where k is the number of iterations and $c \in (0,1)$.

- In general, to achieve $l\left(w^{(k)}\right) - l(w^{*}) \leq \rho$, GD needs $O\left(\frac{1}{\rho}\right)$ iterations;
- With strong convexity, it takes $O\left(\log\left(\frac{1}{\rho}\right)\right)$ siterations[2]

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2: Convex Optimization, S. Boyd & L. Vandenberghe, Ch 9.3

# Why not happy with GD?

- Fast convergence ≠ high efficiency

$$w^{(k)} = w^{(k-1)} - \eta_k \nabla \ell\left(w^{(k-1)}\right) \tag{5}$$

$$= w^{(k-1)} - \eta_k \nabla \left[\frac{1}{n}\sum_{i=1}^{n} \ell_i\left(w^{(k-1)}\right)\right] \tag{6}$$

- Per-iteration complexity = $O(n)$ (extremely large); a single iteration may take forever.
- How to make it cheaper? GD ⇒ SGD





# Stochastic Gradient Decent

Approximate the full gradient via an unbiased estimator

$$w^{(k)} = w^{(k-1)} - \eta_k \nabla\Big(\frac{1}{n}\sum_{i=1}^{n} \ell_i\left(w^{(k-1)}\right)\Big) \tag{7}$$

$$\approx \underbrace{w^{(k-1)} - \eta_k \nabla\Big(\frac{1}{|B|}\sum_{i\in B} \ell_i\left(w^{(k-1)}\right)\Big)}_{\text{mini-batch SGD}^{3}} \quad B \overset{unif}{\sim} \{1, 2, \ldots n\} \tag{8}$$

$$\approx \underbrace{w^{(k-1)} - \eta_k \nabla \ell_i\left(w^{(k-1)}\right)}_{\text{pure SGD}} \quad i \overset{unif}{\sim} \{1, 2, \ldots n\} \tag{9}$$

**Trade-off**: lower computation cost v.s. larger variance

[3] When using GPU, $|B|$ usually depends on the memory budget.

# GD vs SGD

For strongly convex $\ell(w)$, according to [Bottou, 2012]

| **Optimizer** | GD | SGD | Winner |
|---|---|---|---|
| Time per-iteration | $O(n)$ | $O(1)$ | SGD |
| Iterations for accuracy $\rho$ | $O\left(\log\left(\frac{1}{\rho}\right)\right)$ | $\tilde{O}\left(\frac{1}{\rho}\right)$ | GD |
| Time for accuracy $\rho$ | $O\left(n \log \frac{1}{\rho}\right)$ | $\tilde{O}\left(\frac{1}{\rho}\right)$ | Depends |
| Time for test-set error $\epsilon$ | $O\left(\frac{1}{\epsilon^{1/\alpha}} \log \frac{1}{\epsilon}\right)$ | $\tilde{O}\left(\frac{1}{\epsilon}\right)$ | SGD |

where $\frac{1}{2} \leq \alpha \leq 1$





# SVM Solver: Pegasos [Shalev-Shwartz et al., 2011]

$$\ell_i(w) = \max\left(0, 1 - y_i w^\top x_i\right) + \frac{\lambda}{2}\|w\|^2 \tag{10}$$

$$= \begin{cases} \frac{\lambda}{2}\|w\|^2 & y_i w^\top x_i \geq 1 \\ 1 - y_i w^\top x_i + \frac{\lambda}{2}\|w\|^2 & y_i w^\top x_i < 1 \end{cases} \tag{11}$$

Therefore

$$\nabla \ell_i(w) = \begin{cases} \lambda w & y_i w^\top x_i \geq 1 \\ \lambda w - y_i x_i & y_i w^\top x_i < 1 \end{cases} \tag{12}$$

# SVM Solver in 10 Lines

**Algorithm 1:** Pegasos: SGD solver for SVMs

**Input:** $n, \lambda, T$;
**Initialization:** $w \leftarrow 0$;
**for** $k = 1, 2, \ldots, T$ **do**
  $i \overset{uni}{\sim} \{1, 2, \ldots n\}$;
  $\eta_k \leftarrow \frac{1}{\lambda k}$;
  **if** $y_i w^{(k)\top} x_i < 1$ **then**
    $w^{(k+1)} \leftarrow w^{(k)} - \eta_k \left(\lambda w^{(k)} - y_i x_i\right)$
  **else**
    $w^{(k+1)} \leftarrow w^{(k)} - \eta_k \lambda w^{(k)}$
  **end**
**end**
**Output:** $w^{(T+1)}$

$$l_w(x_i, y_i) = \max(0, 1 - y_i w^T x_i) + \frac{\lambda}{2}\|w\|^2$$

$$\frac{dl_w(x_i, y_i)}{dw} = \begin{cases} -x_i y_i + \lambda w & 1 - y_i w^T x_i > 0 \\ \lambda w & otherwise \end{cases}$$





# Empirical Comparison

SGD v.s. batch solvers[4] on RCV1

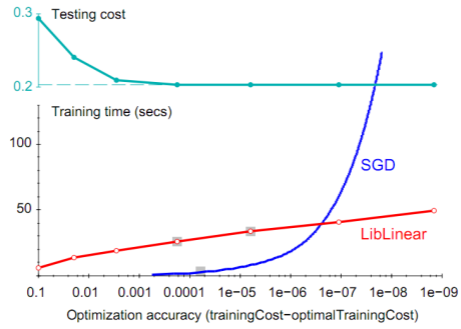
| #Features | #Training examples |
|---|---|
| $47,152$ | $781,265$ |

| Algorithm | Time (secs) | Test Error |
|---|---|---|
| SMO (SVM$^{light}$) | $\approx 16,000$ | 6.02% |
| Cutting Plane (SVM$^{perf}$) | $\approx 45$ | 6.02% |
| SGD | $< 1$ | 6.02% |

What is the magic?

[4] http://leon.bottou.org/projects/sgd

# The Magic




- SGD takes a long time to reach an highly accurate solution on the training data.
- However, for low generalization error (on test data) we may not need the training-set accuracy to be too high.

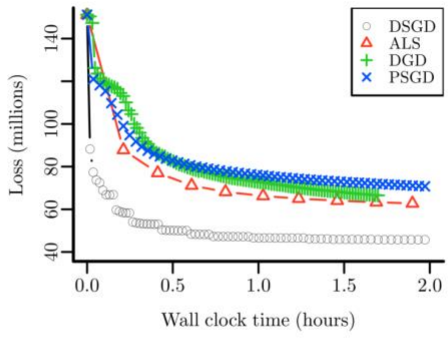
[4] http://leon.bottou.org/slides/largescale/lstut.pdf





# Empirical Results

On Netflix [Gemulla et al., 2011]




DSGD, PSGD: Distributed SGD

ALS: Alternating least squares, one of the state-of-the-art batch solvers

DGD: Distributed GD

## Popular SGD Variants

A non-exhaustive list

1. AdaGrad [Duchi et al., 2011]
2. Momentum [Rumelhart et al., 1988]
3. Nesterov's method [Nesterov et al., 1994]
4. AdaDelta: AdaGrad refined [Zeiler, 2012]
5. Rprop & Rmsprop [Tieleman and Hinton, 2012]
6. Stochastic Variance Reduced Gradient [Johnson and Zhang, 2013]
7. ADAM [Kingma and Ba, 2014]

All are empirically found effective in solving nonconvex problems (e.g., deep neural nets).

Demos [6]: Animation 0, 1, 2, 3

[6] https://www.reddit.com/r/MachineLearning/comments/2gopfa/visualizing_gradient_optimization_techniques/cklhott





## Summarization Remarks

- SGD is extremely handy for large problems.
- It's only one of many handy tools
  - Alternatives: quasi-Newton (BFGS), Coordinate descent, ADMM, CG, etc.
  - How to choose? Depending on the problem structures.

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# Classification

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## Testing-phase Decision Making

- Binary Classification
  - Using one binary classifier to make a yes/no decision for each test instance.
- Multi-label Classification
  - Using K OVA (one-vs-all) classifiers to make an independent yes/no decision per category for each test instance.
- Multi-class Classification
  - Using a multi-class model (e.g., softmax or kNN) to pick one label (out of K) for each test instance.

# Binary Classification Evaluation

(e.g., sentiment classification)

- Given a test set of $n$ instances, the system make $n$ yes/no decisions, as summarized by a two-by-two contingency table

| | $y = 1$ | $y = 0$ | |
|---|---|---|---|
| $\hat{y} = 1$ | a | b | $a + b$ |
| $\hat{y} = 0$ | c | d | $c + d$ |
| | $a + c$ | $b + d$ | $n = a + b + c + d$ |

- Here $a$ (true positive), $b$ (false positive), $c$ (false negative) and $d$ (true negative) are the counts of test instances in the four categories





# Evaluation Metrics for Binary Classifier

- Precision $p = \frac{a}{a+b}$
- Recall $r = \frac{a}{a+c}$
- $F_1$-measure $F_1 = \frac{2pr}{p+r} = \frac{2a}{2a+b+c}$
- Accuracy $Acc = \frac{a+d}{n}$
- Error $Err = \frac{b+c}{n}$

## Why do we prefer $F_1$ over $p$ and $r$?

- A trivial classifier always predicting "yes" for every input will have $r = 100\%$ but is totally useless.
- A trivial classifier always predicting the most popular label without checking the input is totally useless, but would have a high precision, especially when the labels are unbalanced in the data collection.
- $F_1$ is the harmonic average of $p$ and $r$, which means that the $F_1$ value is high only if $p$ and $r$ are both high.





## Harmonic Average

<u>Def.</u> $f(x_1, \cdots, x_n) = \frac{1}{\frac{1}{n}\left(\frac{1}{x_1} + \cdots + \frac{1}{x_n}\right)}$

$F_1(p, r) = \frac{2pr}{r+p} = \frac{1}{\frac{1}{2}\left(\frac{1}{p} + \frac{1}{r}\right)}$ ← Harmonic average of p and r

← Dominated by the smaller one

$F_\beta(p, r) = \frac{(1+\beta^2)pr}{r+\beta^2 p} = \frac{1}{\frac{1}{1+\beta^2}\frac{1}{p} + \frac{\beta^2}{1+\beta^2}\frac{1}{r}}$ ← Weighted harmonic average

# $F_\beta$ with different values of β

$$F_\beta(p,r) = \frac{1}{\frac{1}{1+\beta^2}\frac{1}{p} + \frac{\beta^2}{1+\beta^2}\frac{1}{r}}$$

$$F_{\beta=0} = \frac{1}{\frac{1}{1+0}\frac{1}{p} + \frac{0}{1+0}\frac{1}{r}} = p$$

$$F_{\beta=\infty} = \frac{1}{\frac{1}{1+\infty}\frac{1}{p} + \frac{\infty}{1+\infty}\frac{1}{r}} = r$$

Does $F_{\beta=0.5}$ favor $r$ or p? What about $F_{\beta=2}$ ?





# Multi-class Classification Evaluation

(e.g., OCR word recognition, Amazon product ID, etc.)

- The system assign one and only one label per test instance, which can be summarized using a $K$-by-$K$ confusion matrix M.
- A toy example about 3-way movie classification to the right.
- $Acc = \frac{1}{n}\sum_{k=1}^{K} M_{kk} = \frac{1+70+1}{100} = 72\%$
- $Err = 1 - Acc = 28\%$

| | $y = \text{good}$ | $y = \text{soso}$ | $y = \text{bad}$ | |
|---|---|---|---|---|
| $\hat{y} = \text{good}$ | 1 | 3 | 1 | 5 |
| $\hat{y} = \text{soso}$ | 20 | 70 | 0 | 90 |
| $\hat{y} = \text{bad}$ | 3 | 1 | 1 | 5 |

Confusion Matrix

# Multi-label Classification Evaluation

(e.g., wiki page classification by an OVA model per label)

- For $k = 1, \ 2, \ldots, K,$ construct a contingency table per category as

| | $y_k = 1$ | $y_k = 0$ |
|---|---|---|
| $\hat{y}_k = 1$ | $a_k$ | $b_k$ |
| $\hat{y}_k = 0$ | $c_k$ | $d_k$ |

$$a_k + b_k + c_k + d_k = n$$

- Micro-averaging
  - Merge the $K$ tables into one table by summing the corresponding cells
  - Use the merged table to compute $p, r \ and \ F_1$ (but not $Acc$ or $Err$)
- Macro-averaging
  - Use each of the $K$ tables to compute the category-specific $p, r \ and \ F_1$, then average them over categories as $\bar{p} = \frac{1}{K}\sum_{k=1}^{K} p_k$, and so on.



# Micro-averaging vs. Macro-averaging

- Micro-averaging gives each test instance an equal weight
- Macro-average gives each category an equal weight
- Both are informative for method comparison

# Issues with Accuracy or Error
## (especially for rare categories)

- Consider when the number of labels is large, e.g., $K = 1000$.
- On average, $99.9\%$ of the documents are negative instances for each OVA model.
- Consider a trivial classifier Mr. NO, with the contingency table like

| | $y_k = 1$ | $y_k = 0$ |
|---|---|---|
| $\hat{y}_k = 1$ | $0$ | $0$ |
| $\hat{y}_k = 0$ | $c_k$ | $d_k$ |

$$Acc = \frac{a_k + d_k}{n} = 99.9\%$$

$$Err = \frac{b_k + c_k}{n} = 0.1\%$$

- Take-home message: Focus on $F_1$ (or $F_\beta$) instead.