COMP90051

Workshop Week 04

About the Workshops

- **7** sessions in total
 - **Tue 12:00-13:00 AH211**
 - **Tue 12:00-13:00 AH108 ***
 - **Tue 13:00-14:00 AH210**
 - **Tue 16:15-17:15** AH109
 - **Tue 17:15-18:15 AH236 ***
 - **Tue 18:15-19:15 AH236 ***
 - **Fri** 14:15-15:15 AH211

About the Workshops

Homepage

<u>https://trevorcohn.github.io/comp90051-2017/workshops</u>

□ Solutions will be released on next Friday (a week later).

Syllabus

1	Introduction; Probability theory	Probabilistic models; Parameter fitting	
2	Linear regression; Intro to regularization	Logistic regression; Basis expansion	
3	Optimization; Regularization	Perceptron	\leftarrow
4	Backpropagation	CNNs; Auto-encoders	
5	Hard-margin SVMs	Soft-margin SVMs	
6	Additional topics	Kernel methods	
7	Unsupervised learning	Unsupervised learning	
8	Dimensionality reduction; Principal component analysis	Multidimensional scaling; Spectral clustering	
9	Bayesian fundamentals	Bayesian inference with conjugate priors	
10	PGMs, fundamentals	Conditional independence	
11	PGMs, inference	Belief propagation	
12	Statistical inference; Apps	Subject review	

Outline

Review the lecture, background knowledge, etc.

- Supervised learning as an optimization problem
- Perceptron update rule & loss function
- Logistic regression
 - Predict function
 - Log loss (a.k.a. cross entropy)
- Notebook tasks
 - □ Task 1: Logistic regression
 - □ Task 2: Perceptron classifier

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Supervised learning as an optimization problem

Dataset

- Preprocessing / normalization / feature selection
- Split into train*/test, where test served as the held-out set
 - $\Box Split train* into train/validation (or k folds train/validation, CV)$
- Model / Objective function
 - □ Parameters, solved either analytically or by an optimizer
 - \Box Solved on the training set (or training sets in *k* folds, CV)
 - □ Hyper-parameters, e.g. regularization parameter
 - \Box Selected on the validation set (or validation sets in *k* folds, CV)
- Evaluation on the held-out set

Supervised learning as an optimization problem

Dataset

- Preprocessing / normalization / feature selection
- □ Split into train*/test, where test served as the held-out set
- Model / Objective function
 - **Parameters**, solved either analytically or by an optimizer
 - □ Solved on the training set*

Evaluation on the held-out set

How to solve an optimization problem?

□ Analytic solution \rightarrow solve it by a formula

 $\square \min_{\boldsymbol{w}} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_{2}^{2} + \lambda \|\boldsymbol{w}\|_{2}^{2}, \ \lambda \geq 0 \quad \boldsymbol{\rightarrow} \quad \boldsymbol{w}^{*} = (\boldsymbol{X}^{T}\boldsymbol{X} + \lambda \boldsymbol{I})^{-1}\boldsymbol{X}^{T}\boldsymbol{y}$

 \Box Iterative methods \rightarrow solve it by an optimization algorithm

□ To minimize an objective

Coordinate descent

Gradient-based optimization algorithms (optimizers)

Simplest: gradient descent & stochastic gradient descent

BFGS (in 4a_logistic_regression.ipynb)

□ Many more in packages...

□ To maximize an objective

□ Linear regression has an analytic solution (with L2)

Perceptron has its own update rule

can be interpreted as using stochastic gradient descent (with an appropriate loss function defined)

Gradient-based optimizers can be used for

Linear regression

□ Support vector machines

□ Logistic regression, neural networks

Deep neural networks are usually constructed and optimized using special packages...

Gradient-based optimizers in TensorFlow™

- tf.train.Optimizer
- tf.train.GradientDescentOptimizer
- tf.train.AdadeltaOptimizer
- tf.train.AdagradOptimizer
- tf.train.AdagradDAOptimizer
- tf.train.MomentumOptimizer
- tf.train.AdamOptimizer
- tf.train.FtrlOptimizer
- tf.train.ProximalGradientDescentOptimizer
- tf.train.ProximalAdagradOptimizer
- tf.train.RMSPropOptimizer

https://www.tensorflow.org/api_guides/python/train

Gradient-based optimizers in **PYT**⁶**RCH**

class torch.optim.Optimizer(params, defaults)[source]

class torch.optim.Adadelta(params, Ir=1.0, rho=0.9, eps=1e-06, weight_decay=0)[source]

class torch.optim.Adagrad(params, Ir=0.01, Ir_decay=0, weight_decay=0)[source]

class torch.optim.Adam(params, Ir=0.001, betas=(0.9, 0.999), eps=1e-08, weight_decay=0)[source]

class torch.optim.Adamax(params, Ir=0.002, betas=(0.9, 0.999), eps=1e-08, weight_decay=0)[source]

class torch.optim.ASGD(params, Ir=0.01, lambd=0.0001, alpha=0.75, t0=1000000.0, weight_decay=0)[source]

class torch.optim.LBFGS(params, Ir=1, max_iter=20, max_eval=None, tolerance_grad=1e-05, tolerance_change=1e-09, history_size=100, line_search_fn=None)[source]

class torch.optim.RMSprop(params, Ir=0.01, alpha=0.99, eps=1e-08, weight_decay=0, momentum=0, centered=False)[source]

class torch.optim.Rprop(params, Ir=0.01, etas=(0.5, 1.2), step_sizes=(1e-06, 50))[source]

class torch.optim.SGD(params, Ir=<object object>, momentum=0, dampening=0, weight_decay=0, nesterov=False)[source]

http://pytorch.org/docs/master/optim.html#algorithms COPYRIGHT 2017, THE UNIVERSITY OF MELBOURNE

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Data points

$$x_1 = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} \end{bmatrix} \rightarrow y_1 = +1, \ x_2 = \begin{bmatrix} 1 & x_{2,1} & x_{2,2} \end{bmatrix} \rightarrow y_2 = +1$$

 $x_3 = \begin{bmatrix} 1 & x_{3,1} & x_{3,2} \end{bmatrix} \rightarrow y_3 = -1, x_4 = \begin{bmatrix} 1 & x_{4,1} & x_{4,2} \end{bmatrix} \rightarrow y_4 = -1$

Model parameters

$$\square \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$$

Decision function

 $\Box f(x; w) = xw = x_0w_0 + x_1w_1 + x_2w_2$

 $\square \operatorname{Predict} +1 \operatorname{if} f(\boldsymbol{x}; \boldsymbol{w}) > 0 , \operatorname{predict} -1 \operatorname{if} f(\boldsymbol{x}; \boldsymbol{w}) < 0$

- Iterate over all the points
 - \Box Current point is x_i , and its label is y_i
 - $\Box \text{ Call decision function } s = f(\mathbf{x}_i; \mathbf{w}) = \mathbf{x}_i \mathbf{w}$
 - $\Box \operatorname{Predict} \hat{y}_i \text{ as } +1 \text{ if } s > 0, \text{ as } -1 \text{ if } s < 0$
 - $\Box \text{ If } y_i \neq \hat{y}_i$

$$\Box \text{ If } y_i = +1 \text{ , } \mathbf{w}^{new} = \mathbf{w}^{old} + \mathbf{x}_i^T \text{, or } \begin{cases} w_0^{new} = w_0^{old} + x_{i,0} \\ w_1^{new} = w_1^{old} + x_{i,1} \\ w_2^{new} = w_2^{old} + x_{i,2} \end{cases}$$

$$\Box \text{ If } y_i = -1 \text{ , } \mathbf{w}^{new} = \mathbf{w}^{old} - \mathbf{x}_i^T \text{, } \text{ or } \begin{cases} w_0^{new} = w_0^{old} - x_{i,0} \\ w_1^{new} = w_1^{old} - x_{i,1} \\ w_2^{new} = w_2^{old} - x_{i,2} \end{cases}$$

Suppose x_1 is misclassified

□ This means $y_1 = +1$, $\hat{y}_1 = -1$, $s = f(x_1; w^{old}) = x_1 w^{old} < 0$

Apply the update rule:

 $\Box w^{new} = w^{old} + x_1^T$

□ How does *s* change?

 $\Box s^{new} = x_1 w^{new} = x_1 (w^{old} + x_1^T) = x_1 w^{old} + x_1 x_1^T > s^{old}$

 \Box We hope s > 0 (because $y_1 = +1$)

 \Box After updating w, $s^{new} > s^{old}$, s^{new} may still < 0

 \Box But it improves a bit (at least for x_1)

Suppose x_3 is misclassified

□ This means $y_3 = -1$, $\hat{y}_3 = +1$, $s = f(x_3; w^{old}) = x_3 w^{old} > 0$

Apply the update rule:

 $\Box w^{new} = w^{old} - x_3^T$

□ How does *s* change?

 $\Box s^{new} = x_3 w^{new} = x_3 (w^{old} - x_3^T) = x_3 w^{old} - x_3 x_3^T < s^{old}$

 \Box We hope s < 0 (because $y_3 = -1$)

□ After updating w, $s^{new} < s^{old}$, s^{new} may still > 0

 \Box But it improves a bit (at least for x_3)

A uniform update rule

□ For misclassified positive instance x, y = +1, hope s > 0□ $w^{new} = w^{old} + x^T$ to increase s = f(x; w) = xw

□ For misclassified negative instance x, y = -1, hope s < 0□ $w^{new} = w^{old} - x^T$ to decrease s = f(x; w) = xw

A uniform update rule:

□ For misclassified instance x, $w^{new} = w^{old} + yx^T$ so that □ s = f(x; w) = xw is increased if y = +1□ s = f(x; w) = xw is decreased if y = -1

- Iterate over all the points
 - \Box Current point is x_i , and its label is y_i
 - $\Box \text{ Call decision function } s = f(\mathbf{x}_i; \mathbf{w}) = \mathbf{x}_i \mathbf{w}$
 - $\Box \operatorname{Predict} \hat{y}_i \text{ as } +1 \text{ if } s > 0, \text{ as } -1 \text{ if } s < 0$
 - $\Box \text{ If } y_i \neq \hat{y}_i$

$$\square \mathbf{w}^{new} = \mathbf{w}^{old} + y\mathbf{x}_{i}^{T}, \text{ or } \begin{cases} w_{0}^{new} = w_{0}^{old} + yx_{i,0} \\ w_{1}^{new} = w_{1}^{old} + yx_{i,1} \\ w_{2}^{new} = w_{2}^{old} + yx_{i,2} \end{cases}$$

Iterate over all the points

 \Box Current point is x_i , and its label is y_i

Call decision function $s = f(x_i; w) = x_i w$

 $\square \operatorname{Predict} \hat{y}_i \text{ as } +1 \text{ if } s > 0, \text{ as } -1 \text{ if } s < 0$

 $\Box \text{ If } y_i \neq \hat{y}_i \Leftrightarrow y_i, \hat{y}_i = -1, +1 \text{ or } +1, -1 \Leftrightarrow y_i \hat{y}_i < 0 \Leftrightarrow y_i s < 0$

$$\square \mathbf{w}^{new} = \mathbf{w}^{old} + y\mathbf{x}_{i}^{T}, \text{ or } \begin{cases} w_{0}^{new} = w_{0}^{old} + yx_{i,0} \\ w_{1}^{new} = w_{1}^{old} + yx_{i,1} \\ w_{2}^{new} = w_{2}^{old} + yx_{i,2} \end{cases}$$

Iterate over all the points

 \Box Current point is x_i , and its label is y_i

□ If misclassified ⇔ $yf(\mathbf{x}_i; \mathbf{w}) = y\mathbf{x}_i\mathbf{w} < 0$ □ $\mathbf{w}^{new} = \mathbf{w}^{old} + y\mathbf{x}_i^T$, or $\begin{cases} w_0^{new} = w_0^{old} + yx_{i,0} \\ w_1^{new} = w_1^{old} + yx_{i,1} \\ w_2^{new} = w_2^{old} + yx_{i,2} \end{cases}$

□ The update rule for implementation

□ We can further define a loss function, but only for theoretic analysis.

Define a loss function

□ For misclassified instance x, w^{new} = w^{old} + yx^T so that
□ s = f(x; w) = xw is increased if y = +1
□ s = f(x; w) = xw is decreased if y = -1

Loss functions should be minimized

Define $L(f(\mathbf{x}; \mathbf{w}), y) = -yf(\mathbf{x}; \mathbf{w})$ for misclassified \mathbf{x}

 $\Box -yf(x; w) = -xw$ is decreased if y = +1

 $\Box -yf(x; w) = +xw$ is decreased if y = -1

 \Box So $L(f(\mathbf{x}; \mathbf{w}), \mathbf{y}) = -yf(\mathbf{x}; \mathbf{w})$ decreases after updating \mathbf{w}

Gradient of the loss function

 $\Box L(f(x; w), y) = -yf(x; w) = -y(x_0w_0 + x_1w_1 + x_2w_2)$

$$\frac{\partial L}{\partial w_0} = -yx_0 \quad \frac{\partial L}{\partial w_1} = -yx_1 \quad \frac{\partial L}{\partial w_2} = -yx_2$$

$$\frac{\partial L}{\partial \boldsymbol{w}} = \begin{bmatrix} \frac{\partial L}{\partial w_0} \\ \frac{\partial L}{\partial w_1} \\ \frac{\partial W_1}{\partial L} \\ \frac{\partial L}{\partial w_2} \end{bmatrix} = -y \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = -y \boldsymbol{x}^T$$

The uniform update rule

 \Box For misclassified instance x, $w^{new} = w^{old} + yx^T$

□ For misclassified instance *x*, the loss function is defined as L(f(x; w), y) = -yf(x; w) $\frac{\partial L}{\partial w} = -yx^T$

□ So the update rule can be written as

$$\boldsymbol{w}^{new} = \boldsymbol{w}^{old} + y\boldsymbol{x}^{T} = \boldsymbol{w}^{old} - \frac{\partial L}{\partial \boldsymbol{w}}$$

Define $L(f(\mathbf{x}; \mathbf{w}), y) = -yf(\mathbf{x}; \mathbf{w})$ for misclassified instances

□ Iterate over all the points

 \Box Current point is x_i , and its label is y_i

 $\Box \text{ If misclassified} \Leftrightarrow yf(\mathbf{x}_i; \mathbf{w}) = y\mathbf{x}_i\mathbf{w} < 0 \Leftrightarrow L(f(\mathbf{x}; \mathbf{w}), y) > 0$

$$\boldsymbol{w}^{new} = \boldsymbol{w}^{old} - \frac{\partial L}{\partial \boldsymbol{w}}$$

Perceptron \rightarrow stochastic gradient descent

Define

$$L(f(\mathbf{x}; \mathbf{w}), y) = \begin{cases} -yf(\mathbf{x}; \mathbf{w}) & \text{if } L(f(\mathbf{x}; \mathbf{w}), y) > 0 \Leftrightarrow \text{misclassified} \\ 0 & \text{otherwise} \end{cases}$$

🖵 Then

$$\frac{\partial L}{\partial \boldsymbol{w}} = \begin{cases} -y\boldsymbol{x}^T & \text{if } L(f(\boldsymbol{x};\boldsymbol{w}),\boldsymbol{y}) > 0 \Leftrightarrow \text{misclassified} \\ \boldsymbol{0} & otherwise \end{cases}$$

□ Iterate over all the points

 \Box Current point is x_i , and its label is y_i

Apply the update rule

$$\boldsymbol{w}^{new} = \boldsymbol{w}^{old} - \frac{\partial L}{\partial \boldsymbol{w}}$$

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Logistic regression (2-D points, 3 classes)

Data points

$$x_1 = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} \end{bmatrix} \rightarrow y_1 = 0, \ x_2 = \begin{bmatrix} 1 & x_{2,1} & x_{2,2} \end{bmatrix} \rightarrow y_2 = 1$$

 $\Box x_3 = \begin{bmatrix} 1 & x_{3,1} & x_{3,2} \end{bmatrix} \rightarrow y_3 = 2, x_4 = \begin{bmatrix} 1 & x_{4,1} & x_{4,2} \end{bmatrix} \rightarrow y_4 = 2$

Model parameters

$$\square W = \begin{bmatrix} w_0 & w_1 & w_2 \end{bmatrix} = \begin{bmatrix} w_{0,0} & w_{0,1} & w_{0,2} \\ w_{1,0} & w_{1,1} & w_{1,2} \\ w_{2,0} & w_{2,1} & w_{2,2} \end{bmatrix}$$

 \Box Decision function, predict \boldsymbol{x} as class j if s_j is the largest.

$$\Box f(\mathbf{x}; \mathbf{w}) = \mathbf{x}\mathbf{W} = \begin{bmatrix} \mathbf{x}\mathbf{w}_0 \\ \mathbf{x}\mathbf{w}_1 \\ \mathbf{x}\mathbf{w}_2 \end{bmatrix}^T = \begin{bmatrix} x_0w_{0,0} + x_1w_{1,0} + x_2w_{2,0} \\ x_0w_{0,1} + x_1w_{1,1} + x_2w_{2,1} \\ x_0w_{0,2} + x_1w_{1,2} + x_2w_{2,2} \end{bmatrix}^T = \begin{bmatrix} s_0 \\ s_1 \\ s_2 \end{bmatrix}^T$$

Logistic regression (2-D points, 3 classes)

Model parameters

$$\square W = \begin{bmatrix} w_0 & w_1 & w_2 \end{bmatrix} = \begin{bmatrix} w_{0,0} & w_{0,1} & w_{0,2} \\ w_{1,0} & w_{1,1} & w_{1,2} \\ w_{2,0} & w_{2,1} & w_{2,2} \end{bmatrix}$$

 \Box Decision function, predict \boldsymbol{x} as class j if s_j is the largest.

$$\Box f(\mathbf{x}; \mathbf{w}) = \mathbf{x}\mathbf{W} = \begin{bmatrix} \mathbf{x}\mathbf{w}_0 \\ \mathbf{x}\mathbf{w}_1 \\ \mathbf{x}\mathbf{w}_2 \end{bmatrix}^T = \begin{bmatrix} x_0w_{0,0} + x_1w_{1,0} + x_2w_{2,0} \\ x_0w_{0,1} + x_1w_{1,1} + x_2w_{2,1} \\ x_0w_{0,2} + x_1w_{1,2} + x_2w_{2,2} \end{bmatrix}^T = \begin{bmatrix} s_0 \\ s_1 \\ s_2 \end{bmatrix}^T$$

Output the distribution

$$\square p(y|\mathbf{x}; \mathbf{W}) = \frac{1}{e^{s_0} + e^{s_1} + e^{s_2}} [e^{s_0} \quad e^{s_1} \quad e^{s_2}] \propto [e^{s_0} \quad e^{s_1} \quad e^{s_2}]$$

Logistic regression (2-D points, 3 classes)

 \Box Decision function, predict x as class j if s_j is the largest.

$$\Box f(\mathbf{x}; \mathbf{w}) = \mathbf{x}\mathbf{W} = \begin{bmatrix} \mathbf{x}\mathbf{w}_0 \\ \mathbf{x}\mathbf{w}_1 \\ \mathbf{x}\mathbf{w}_2 \end{bmatrix}^T = \begin{bmatrix} x_0w_{0,0} + x_1w_{1,0} + x_2w_{2,0} \\ x_0w_{0,1} + x_1w_{1,1} + x_2w_{2,1} \\ x_0w_{0,2} + x_1w_{1,2} + x_2w_{2,2} \end{bmatrix}^T = \begin{bmatrix} s_0 \\ s_1 \\ s_2 \end{bmatrix}^T$$

Output the distribution

$$p(y|\mathbf{x}; \mathbf{W}) = \frac{1}{e^{s_0} + e^{s_1} + e^{s_2}} [e^{s_0} e^{s_1} e^{s_2}] \propto [e^{s_0} e^{s_1} e^{s_2}]$$

The log-loss
$$L(\mathbf{x}_i, y_i; \mathbf{W}) = -\log p(y = y_i | \mathbf{x} = \mathbf{x}_i; \mathbf{W}) = -\log \frac{e^{s_{y_i}}}{e^{s_0} + e^{s_1} + e^{s_2}}$$
$$= -s_{y_i} + \log(e^{s_0} + e^{s_1} + e^{s_2})$$

Log-loss for each data point & mean loss

i	y _i	$p(y = j \boldsymbol{x} = \boldsymbol{x}_i, \boldsymbol{W})$			log-loss
L		j = 0	j = 1	<i>j</i> = 2	108-1035
1	0	0.6	0.3	0.1	
2	1	0.2	0.7	0.1	
3	2	0.5	0.3	0.2	
4	2	0.3	0.3	0.4	

Log-loss for each data point & mean loss

i	y _i	$p(y = j \boldsymbol{x} = \boldsymbol{x}_i, \boldsymbol{W})$			
L		j = 0	j = 1	<i>j</i> = 2	log-loss
1	0	0.6	0.3	0.1	-log 0.6
2	1	0.2	0.7	0.1	$-\log 0.7$
3	2	0.5	0.3	0.2	-log 0.2
4	2	0.3	0.3	0.4	-log 0.4

□ Mean loss (without regularization)

$$L = \frac{1}{4} \sum_{i=1}^{4} -\log p(y = y_i | \mathbf{x} = \mathbf{x}_i; \mathbf{W})$$
$$= -\frac{1}{4} (\log 0.6 + \log 0.7 + \log 0.2 + \log 0.4)$$

Log-loss for each data point & mean loss

i	y _i	$p(y = j \boldsymbol{x} = \boldsymbol{x}_i, \boldsymbol{W})$			
L		j = 0	j = 1	<i>j</i> = 2	↓ log-loss
1	0	0.6 1	0.3	0.1	-log 0.6
2	1	0.2	0.7↑	0.1	-log 0.7
3	2	0.5	0.3	0.2 1	-log 0.2
4	2	0.3	0.3	0.4 1	-log 0.4

□ Mean loss (without regularization)

$$L = \frac{1}{4} \sum_{i=1}^{4} -\log p(y = y_i | \mathbf{x} = \mathbf{x}_i; \mathbf{W})$$

= $-\frac{1}{4} (\log 0.6 + \log 0.7 + \log 0.2 + \log 0.4)$

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Notebook tasks

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