10-605/805 – ML for Large Datasets Lecture 6: Distributed PCA & Logistic Regression

Front Matter

- Recitation 3 on 9/16 will go over HW1 solutions
- HW2 released 9/8, due 9/22 at 11:59 PM

Recall: PCA Algorithm

- Input: $\mathcal{D} = \left\{ \left(\mathbf{x}^{(i)} \right) \right\}_{i=1}^n$, r
- 1. Center the data
 - A. Optionally, normalize the data by features so that all features are of the same scale
- 2. Compute the covariance matrix $C_X = X^T X$
- 3. Collect the top r eigenvectors (corresponding to the r largest eigenvalues), $P \in \mathbb{R}^{k \times r}$
- 4. Project the data into the space defined by P, Z = XP

Recall: Computational Cost of PCA

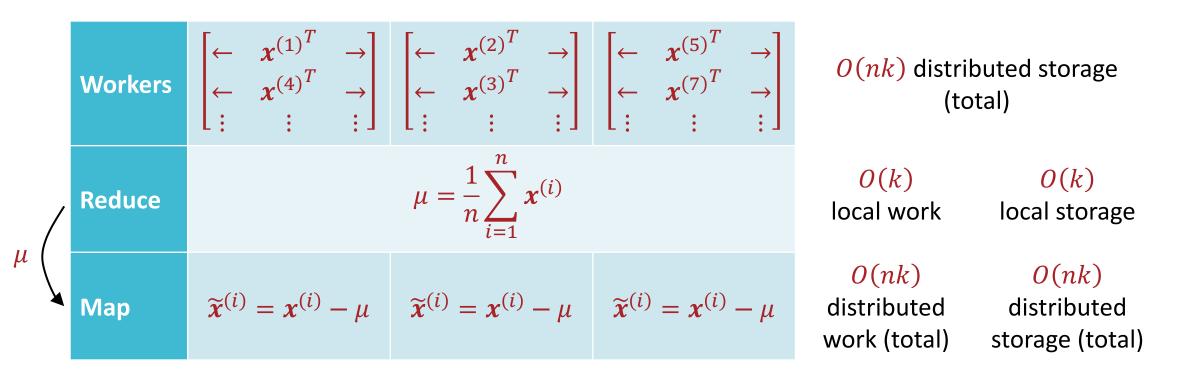
• Input:
$$\mathcal{D} = \left\{ \left(\mathbf{x}^{(i)} \right) \right\}_{i=1}^n$$
, r

- 1. Center the data
 - A. Optionally, normalize the data by features so that all features are of the same scale
- 2. Compute the covariance matrix $C_X = X^T X (O(nk^2))$
- 3. Collect the top r eigenvectors (corresponding to the r largest eigenvalues), $P \in \mathbb{R}^{k \times r}$ ($O(k^3)$)
- 4. Project the data into the space defined by P, Z = XP (O(nkr))

PCA: Large n, Small k

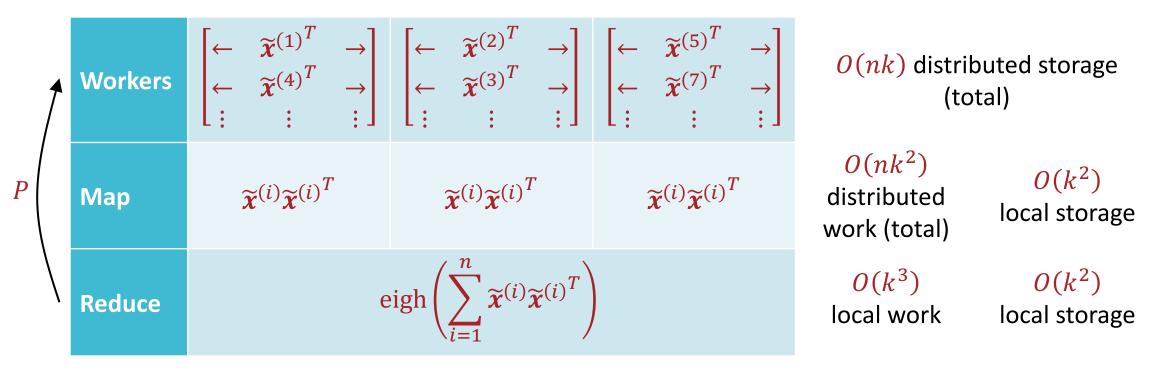
- Assume $O(k^3)$ computation and $O(k^2)$ storage is possible on a single machine
 - ✓ We can store and compute the eigenvalues of X^TX We cannot compute X^TX We cannot store X

- Approach: basically the same as distributed linear regression
 - 1. Center the data in a distributed way
 - 2. Store the rows of X across different machines
 - 3. Compute X^TX as the sum of outer products



O(k) communication

Distributed Centering of the Data



O(kr) communication

Distributed Eigendecomposition of X^TX

Workers	[← ← ::	$\widetilde{\boldsymbol{x}}^{(1)^T}$ $\widetilde{\boldsymbol{x}}^{(4)^T}$ \vdots	$\begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \\ \vdots \end{array}$	[← ← :	$\widetilde{\boldsymbol{x}}^{(2)^T}$ $\widetilde{\boldsymbol{x}}^{(3)^T}$ \vdots	$\begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \\ \vdots \end{array}$	← ← ÷	$\widetilde{x}^{(5)^T}$ $\widetilde{x}^{(7)^T}$ \vdots	$\begin{array}{c} \rightarrow \\ \rightarrow \\ \vdots \end{array}$
Мар	$P\widetilde{m{x}}^{(i)}$		$P\widetilde{\boldsymbol{x}}^{(i)}$			$P\widetilde{\boldsymbol{\chi}}^{(i)}$			

O(nk) distributed storage (total)

O(nkr)
distributed
work (total)

O(nr) local storage

Distributed Computation of PCA Scores

PCA: Large n, Large k

• Now, $O(k^3)$ computation and $O(k^2)$ storage is *not* possible on a single machine

We cannot store and compute the eigenvalues of X^TX

We cannot compute X^TX

We cannot store X

- Idea: use a different algorithm!
 - Turn to an iterative method for computing eigenvectors

PCA: Large n, Large k

• Now, $O(k^3)$ computation and $O(k^2)$ storage is *not* possible on a single machine

We cannot store and compute the eigenvalues of X^TX

We cannot compute X^TX

We cannot store X

- Idea: use a different algorithm!
 - Turn to an iterative method for computing eigenvectors the eigenvector associated with the largest eigenvalue $(r=1) \rightarrow \text{power iteration}$

• Fact: $A = X^T X$ is "diagonalizable", i.e., any k-dimensional vector can be written as a linear combination of A's eigenvectors:

$$\boldsymbol{b} = c_1 \boldsymbol{v}_1 + c_2 \boldsymbol{v}_2 \dots + c_k \boldsymbol{v}_k$$

• This follows because X^TX is real and symmetric

• Assume $A = X^T X$ has one eigenvalue that is strictly larger than the others:

$$\lambda_1 > \lambda_2 \geq \dots \geq \lambda_k$$

- Input: $A = X^T X$
- Initialize $b^{(0)}$ to all zeros and set t=0
- 1. While TERMINATION CRITERION is not satisfied
 - a. Update the vector **b**:

$$\boldsymbol{b}^{(t+1)} \leftarrow \frac{A\boldsymbol{b}^{(t)}}{\|A\boldsymbol{b}^{(t)}\|_{2}}$$

- b. Increment $t: t \leftarrow t + 1$
- Output: $b^{(t)}$, the eigenvector corresponding to the largest eigenvalue of A!

$$\mathbf{b}^{(0)} = c_{1}\mathbf{v}_{1} + c_{2}\mathbf{v}_{2} + \dots + c_{k}\mathbf{v}_{k}$$

$$A\mathbf{b}^{(0)} = c_{1}A\mathbf{v}_{1} + c_{2}A\mathbf{v}_{2} + \dots + c_{k}A\mathbf{v}_{k}$$

$$= c_{1}\lambda_{1}\mathbf{v}_{1} + c_{2}\lambda_{2}\mathbf{v}_{2} + \dots + c_{k}\lambda_{k}\mathbf{v}_{k}$$

$$A(A\mathbf{b}^{(0)}) = (A)^{2}\mathbf{b}^{(0)} = c_{1}\lambda_{1}A\mathbf{v}_{1} + c_{2}\lambda_{2}A\mathbf{v}_{2} + \dots + c_{k}\lambda_{k}A\mathbf{v}_{k}$$

$$= c_{1}\lambda_{1}^{2}\mathbf{v}_{1} + c_{2}\lambda_{2}^{2}\mathbf{v}_{2} + \dots + c_{k}\lambda_{k}^{2}\mathbf{v}_{k}$$

$$(A)^{t}\mathbf{b}^{(0)} = c_{1}\lambda_{1}^{t}\mathbf{v}_{1} + c_{2}\lambda_{2}^{t}\mathbf{v}_{2} + \dots + c_{k}\lambda_{k}^{t}\mathbf{v}_{k}$$

$$= c_{1}\lambda_{1}^{t}\left(\mathbf{v}_{1} + c_{2}\left(\frac{\lambda_{2}}{\lambda_{1}}\right)^{t}\mathbf{v}_{2} \dots + c_{2}\left(\frac{\lambda_{k}}{\lambda_{1}}\right)^{t}\mathbf{v}_{k}\right)$$

$$\to c_{1}\lambda_{1}^{t}(\mathbf{v}_{1}) \text{ as } t \to \infty$$

Normalize $(A)^t b^{(0)}$ to have unit norm: $b^{(t)} = \frac{(A)^t b^{(0)}}{\|(A)^t b^{(0)}\|_2}$

- Input: $A = X^T X$
- Initialize $b^{(0)}$ to all zeros and set t=0
- While TERMINATION CRITERION is not satisfied
 - a. Update the vector **b**:

$$\boldsymbol{b}^{(t+1)} \leftarrow \frac{\boldsymbol{X}^T \boldsymbol{X} \boldsymbol{b}^{(t)}}{\left\| \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{b}^{(t)} \right\|_2}$$

- b. Increment $t: t \leftarrow t + 1$
- Output: $b^{(t)}$, the eigenvector corresponding to the largest eigenvalue of A!

- Input: $A = X^T X$
- Initialize $\boldsymbol{b}^{(0)}$ to all zeros and set t=0
- While TERMINATION CRITERION is not satisfied
 - a. Update the vector **b** using some intermediate steps:

$$\boldsymbol{b}^{(t+1)} \leftarrow X^T X \boldsymbol{b}^{(t)} = \left(\sum_{i=1}^n \widetilde{\boldsymbol{x}}^{(i)} \widetilde{\boldsymbol{x}}^{(i)}^T\right) \boldsymbol{b}^{(t)}$$

$$\boldsymbol{b}^{(t+1)} \leftarrow \frac{\boldsymbol{b}^{(t+1)}}{\left\|\boldsymbol{b}^{(t+1)}\right\|_2}$$

- b. Increment $t: t \leftarrow t + 1$
- Output: $b^{(t)}$, the eigenvector corresponding to the largest eigenvalue of A!

- Input: $A = X^T X$
- Initialize $\boldsymbol{b}^{(0)}$ to all zeros and set t=0
- While TERMINATION CRITERION is not satisfied
 - a. Update the vector **b** using some intermediate steps:

$$\boldsymbol{b}^{(t+1)} \leftarrow X^T X \boldsymbol{b}^{(t)} = \sum_{i=1}^n \widetilde{\boldsymbol{x}}^{(i)} \left(\widetilde{\boldsymbol{x}}^{(i)}^T \boldsymbol{b}^{(t)} \right)$$

$$\boldsymbol{b}^{(t+1)} \leftarrow \frac{\boldsymbol{b}^{(t+1)}}{\left\|\boldsymbol{b}^{(t+1)}\right\|_{2}}$$

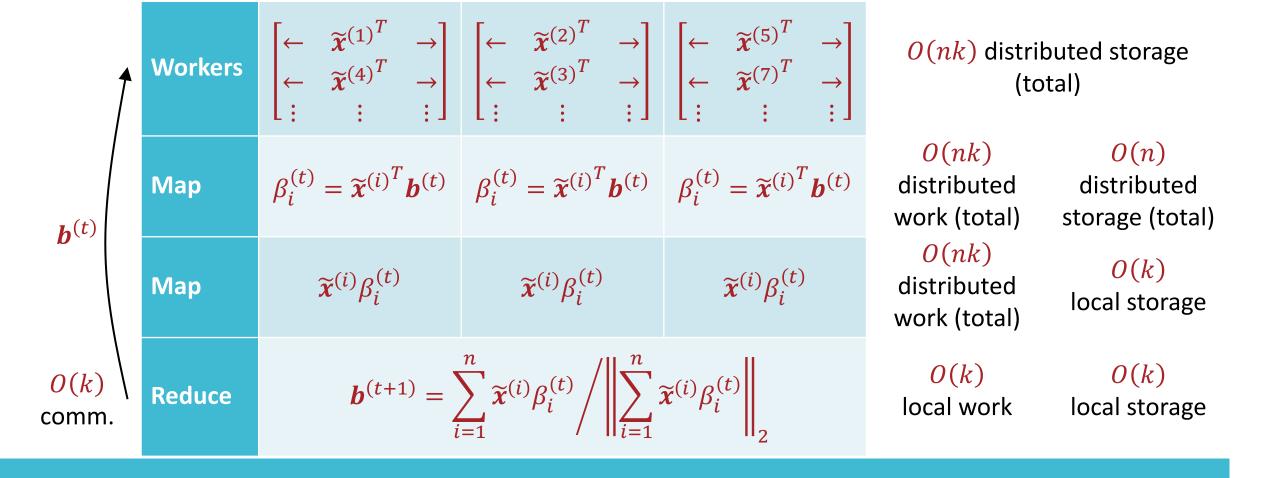
- b. Increment $t: t \leftarrow t + 1$
- Output: $b^{(t)}$, the eigenvector corresponding to the largest eigenvalue of A!

- Input: $A = X^T X$
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- While TERMINATION CRITERION is not satisfied
 - a. Update the vector **b** using some intermediate steps:

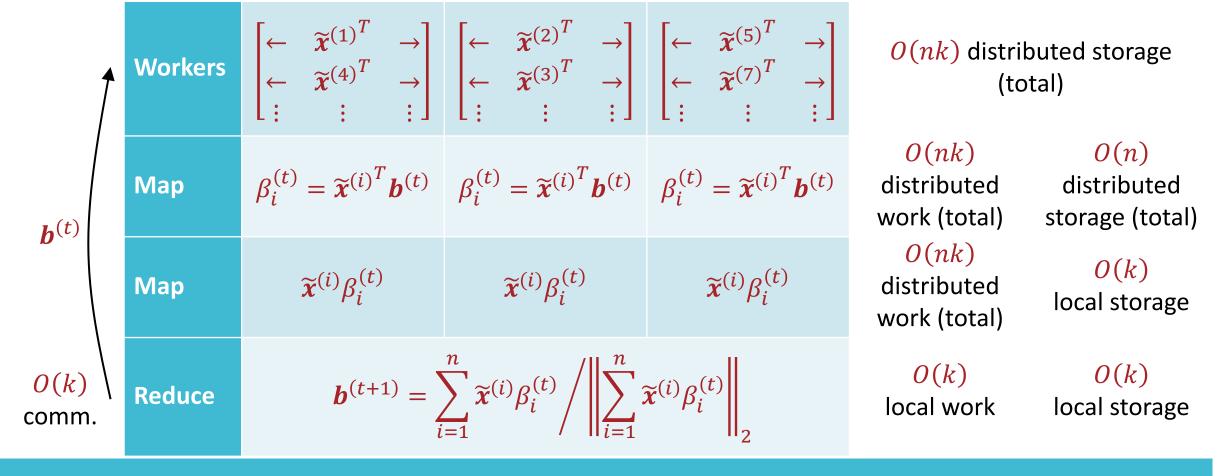
$$\boldsymbol{b}^{(t+1)} \leftarrow X^T X \boldsymbol{b}^{(t)} = \sum_{i=1}^n \widetilde{\boldsymbol{x}}^{(i)} \left(\beta_i^{(t)} \right)$$

$$\boldsymbol{b}^{(t+1)} \leftarrow \frac{\boldsymbol{b}^{(t+1)}}{\left\|\boldsymbol{b}^{(t+1)}\right\|_{2}}$$

- b. Increment $t: t \leftarrow t + 1$
- Output: $b^{(t)}$, the eigenvector corresponding to the largest eigenvalue of A!



Distributed Power Iteration



Disclaimer: to find more than one eigenvector, we need to use similar (but slightly more complicated methods), e.g., PySpark's MLlib uses Krylov subspace methods

Background: Empirical Risk Minimization

- A common framework for supervised learning
- Given:
 - some labelled training dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^n$
 - a loss function ℓ : $\mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$
 - $oldsymbol{\cdot}$ a hypothesis class or set of functions $oldsymbol{\mathcal{F}}$

the goal is to find

$$\hat{f} = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \sum_{i=1}^{n} \ell(f(\mathbf{x}^{(i)}), y^{(i)})$$

with the hope that

$$\mathbb{E}_{p(\mathbf{x},y)}[\ell(f(\mathbf{x}),y)] \approx \sum_{i=1}^{n} \ell(f(\mathbf{x}^{(i)}),y^{(i)})$$

Background: Binary Classification

- A type of supervised learning
- Given:
 - some labelled training dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^n$
 - a loss function $\ell: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ where $\mathcal{Y} = \{0,1\}$
 - $oldsymbol{\cdot}$ a hypothesis class or set of functions $oldsymbol{\mathcal{F}}$

the goal is to find

$$\hat{f} = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \sum_{i=1}^{n} \ell(f(\mathbf{x}^{(i)}), y^{(i)})$$

Background: Binary Classification w/ 0-1 Loss

- A type of supervised learning
- Given:
 - some labelled training dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^n$
 - $\ell(y, y') = 1(y \neq y')$ for $y, y' \in \{0, 1\}$
 - $oldsymbol{\cdot}$ a hypothesis class or set of functions ${\mathcal F}$

the goal is to find

$$\hat{f} = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \sum_{i=1}^{n} \ell(f(\mathbf{x}^{(i)}), y^{(i)})$$

• This loss function is difficult to optimize (non-convex)...

A Probabilistic Approach to Binary Classification

- Suppose we have binary labels $y \in \{0,1\}$ and D-dimensional inputs $\mathbf{x} = [1, x_1, ..., x_D]^T \in \mathbb{R}^{D+1}$
- Assume

$$P(Y = 1|\mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$$
$$= \frac{\exp(\mathbf{w}^T \mathbf{x})}{\exp(\mathbf{w}^T \mathbf{x}) + 1}$$

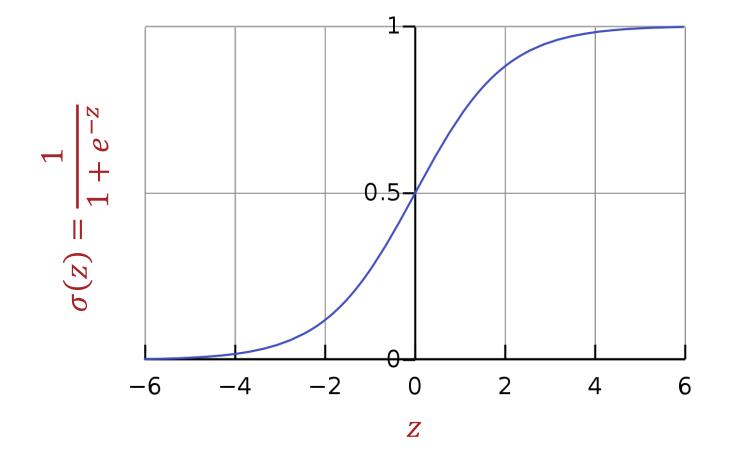
This implies two useful facts:

1.
$$P(Y = 0|x) = 1 - P(Y = 1|x) = \frac{1}{\exp(w^T x) + 1}$$

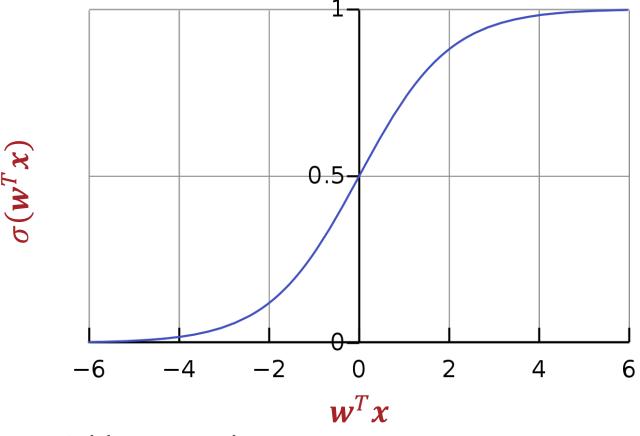
2. $\frac{P(Y = 1|x)}{P(Y = 0|x)} = \exp(w^T x) \rightarrow \log \frac{P(Y = 1|x)}{P(Y = 0|x)} = w^T x$

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Logistic Function



Why use the Logistic Function?



- Differentiable everywhere
- σ : $\mathbb{R} \rightarrow [0, 1]$
- The decision boundary is linear in x!

Logistic Regression Decision Boundary

$$y' = \begin{cases} 1 \text{ if } P(Y = 1 | x) \ge \frac{1}{2} \\ 0 \text{ otherwise} \end{cases}$$

$$P(Y = 1 | x) = \sigma(\mathbf{w}^T x) = \frac{1}{1 + \exp(-\mathbf{w}^T x)} \ge \frac{1}{2}$$

$$2 \ge 1 + \exp(-\mathbf{w}^T x)$$

$$1 \ge \exp(-\mathbf{w}^T x)$$

$$\log(1) \ge -\mathbf{w}^T x$$

$$0 \le \mathbf{w}^T x$$

Why 1/2?

$$y' = \begin{cases} 1 \text{ if } P(Y = 1 | x) \ge \frac{1}{2} \\ 0 \text{ otherwise} \end{cases}$$

Therefore
$$P(Y = 1 | x) = \sigma(w^T x) = \frac{1}{1 + \exp(-w^T x)} \ge \frac{1}{2}$$

$$2 \ge 1 + \exp(-w^T x)$$

$$1 \ge \exp(-w^T x)$$

$$\log(1) \ge -w^T x$$

$$0 \le w^T x$$

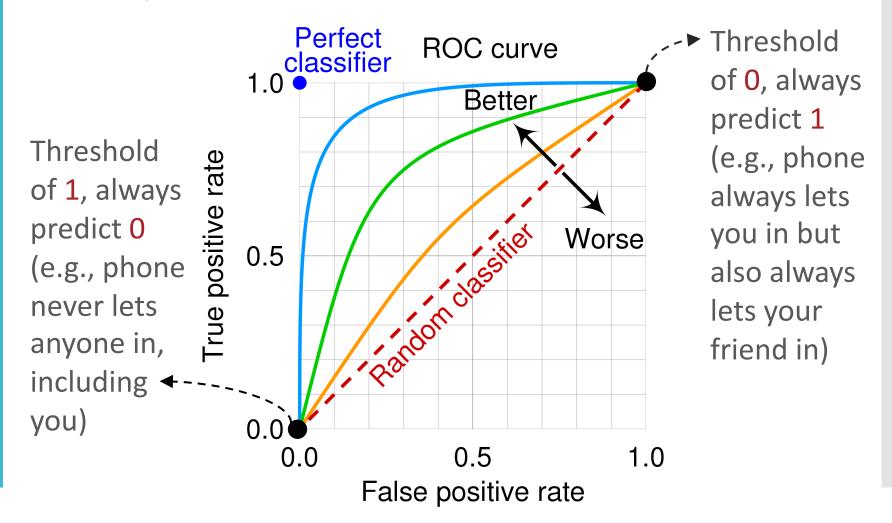
Aside: Different Kinds of Errors

		y					
		0	1				
ν'	0	True negative (TN)	False negative (FN)				
	1	False positive (FP)	True positive (TP)				

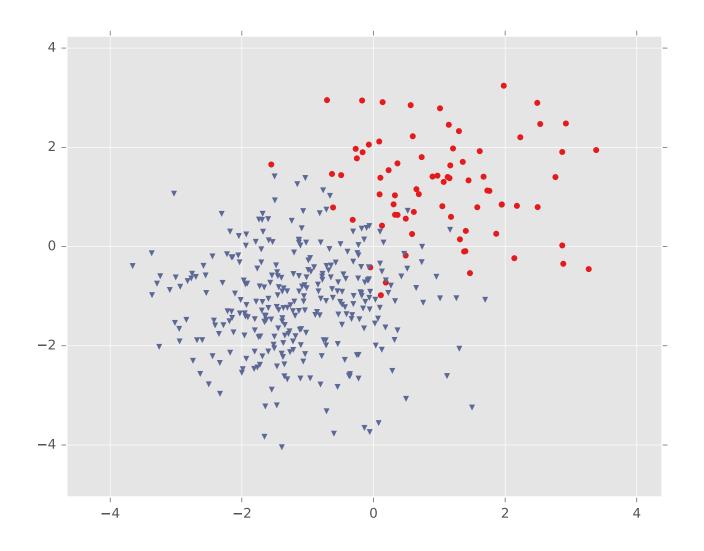
- Depending on the setting, these kinds of errors can have wildly different impacts/costs, e.g., facial recognition for unlocking phones:
 - False negative = minor nuisance, just try again
 - False positive = major security breach
 - Using a threshold > 1/2 will tend to decrease the number of false positives

Aside: Receiver Operating Characteristic (ROC) Curves

 Plots true positive rate, TPR = TP / (TP + FN), against false positive rate, FPR = FP / (FP + TN)

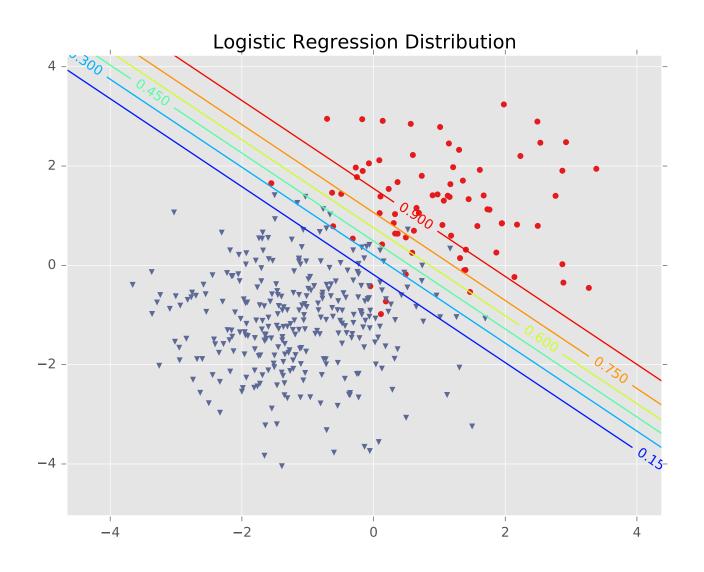


Logistic Regression: Decision Boundary



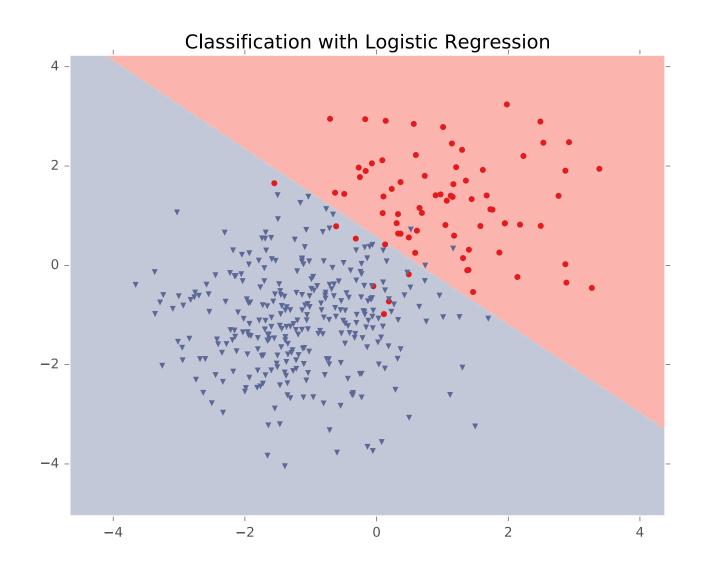
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Logistic Regression: Decision Boundary



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Logistic Regression: Decision Boundary



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Logistic Regression: Setting the Parameters

 Goal: find the w that maximizes the (conditional) probability of the training dataset:

$$\prod_{i=1}^{n} P(y^{(i)}|\mathbf{x}^{(i)},\mathbf{w})$$

• This is equivalent to finding the **w** that *minimizes* the negative log of this probability:

$$L_{\mathcal{D}}(\mathbf{w}) = -\log \prod_{i=1}^{n} P(y^{(i)} | \mathbf{x}^{(i)}, \mathbf{w})$$

$$= -\log \prod_{i=1}^{n} P(Y = 1 | \mathbf{x}^{(i)}, \mathbf{w})^{y^{(i)}} (P(Y = 0 | \mathbf{x}^{(i)}, \mathbf{w}))^{1-y^{(i)}}$$

$$= -\sum_{i=1}^{n} y^{(i)} \log P(Y = 1 | \mathbf{x}^{(i)}, \mathbf{w}) + (1 - y^{(i)}) \log P(Y = 0 | \mathbf{x}^{(i)}, \mathbf{w})$$

Logistic Regression as Empirical Risk Minimization

- A type of supervised learning
- Given:
 - some labelled training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}_{i=1}^n$
 - the log loss
 - \mathcal{F} = the set of all linear decision boundaries

the goal is to find

$$\underset{w}{\operatorname{argmin}} - \sum_{i=1}^{n} (y^{(i)} \log P(Y = 1 | \mathbf{x}^{(i)}, \mathbf{w})) + (1 - y^{(i)}) \log P(Y = 0 | \mathbf{x}^{(i)}, \mathbf{w})$$

$$= \underset{w}{\operatorname{argmin}} - \sum_{i=1}^{n} y^{(i)} \log \frac{P(Y=1|\mathbf{x}^{(i)}, \mathbf{w})}{P(Y=0|\mathbf{x}^{(i)}, \mathbf{w})} + \log P(Y=0|\mathbf{x}^{(i)}, \mathbf{w})$$

=
$$\underset{w}{\operatorname{argmin}} - \sum_{i=1}^{n} y^{(i)} w^{T} x^{(i)} - \log (1 + \exp(w^{T} x^{(i)}))$$

Logistic Regression as Empirical Risk Minimization

$$L_{D}(\mathbf{w}) = -\sum_{i=1}^{n} y^{(i)} \mathbf{w}^{T} \mathbf{x}^{(i)} - \log\left(1 + \exp(\mathbf{w}^{T} \mathbf{x}^{(i)})\right)$$

$$\nabla_{\mathbf{w}} L_{D}(\mathbf{w}) = -\sum_{i=1}^{n} y^{(i)} \nabla_{\mathbf{w}} \mathbf{w}^{T} \mathbf{x}^{(i)} - \nabla_{\mathbf{w}} \log\left(1 + \exp(\mathbf{w}^{T} \mathbf{x}^{(i)})\right)$$

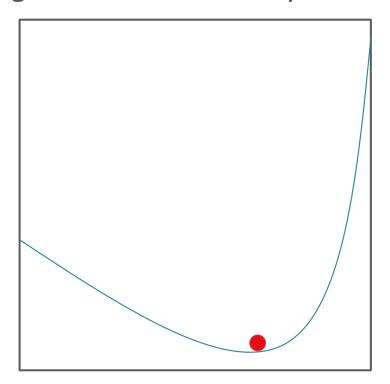
$$= -\sum_{i=1}^{n} y^{(i)} \mathbf{x}^{(i)} - \frac{\exp(\mathbf{w}^{T} \mathbf{x}^{(i)})}{1 + \exp(\mathbf{w}^{T} \mathbf{x}^{(i)})} \mathbf{x}^{(i)}$$

$$= \sum_{i=1}^{n} \mathbf{x}^{(i)} \frac{1}{\exp(-\mathbf{w}^{T} \mathbf{x}^{(i)}) + 1} - y^{(i)} \mathbf{x}^{(i)}$$

$$= \sum_{i=1}^{n} \mathbf{x}^{(i)} \left(\sigma(\mathbf{w}^{T} \mathbf{x}^{(i)}) - y^{(i)}\right)$$

Recall: Gradient Descent

- An iterative method for minimizing functions
- Requires the gradient to exist everywhere



Good news: the log loss for logistic regression is convex!

Gradient Descent for Logistic Regression

• Input:
$$\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^n, \alpha$$

- 1. Initialize $\mathbf{w}^{(0)}$ to all zeros and set t=0
- 2. While TERMINATION CRITERION is not satisfied
 - a. Compute the gradient:

$$\nabla_{\boldsymbol{w}} L_{\mathcal{D}}\left(\boldsymbol{w}^{(t)}\right) = \sum_{i=1}^{n} \boldsymbol{x}^{(i)} \left(\operatorname{logit}\left(\boldsymbol{w}^{(t)^{T}} \boldsymbol{x}^{(i)}\right) - \boldsymbol{y}^{(i)} \right)$$

- b. Update $w: w^{(t+1)} \leftarrow w^{(t)} \alpha \nabla_w L_{\mathcal{D}}(w^{(t)})$
- c. Increment $t: t \leftarrow t + 1$
- Output: $\mathbf{w}^{(t)}$

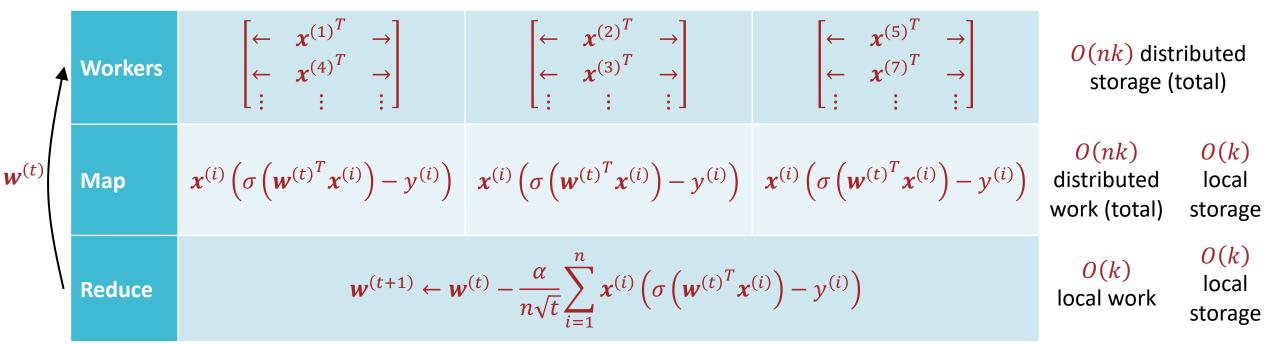
Idea: distribute $x^{(i)}$ and compute summands in parallel

• Input:
$$\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^n, \alpha$$

- 1. Initialize $\mathbf{w}^{(0)}$ to all zeros and set t=0
- While TERMINATION CRITERION is not satisfied
 - a. Compute the gradient:

$$\nabla_{\mathbf{w}} L_{\mathcal{D}}\left(\mathbf{w}^{(t)}\right) = \sum_{i=1}^{n} \mathbf{x}^{(i)} \left(\operatorname{logit}\left(\mathbf{w}^{(t)^{T}} \mathbf{x}^{(i)}\right) - \mathbf{y}^{(i)} \right)$$

- b. Update $w: w^{(t+1)} \leftarrow w^{(t)} \alpha \nabla_w L_{\mathcal{D}}(w^{(t)})$
- c. Increment $t: t \leftarrow t + 1$
- Output: $\mathbf{w}^{(t)}$



O(k) communication

Distributed Gradient Descent for Logistic Regression

What do linear regression, PCA and logistic regression all have in common?

- They're all linear methods...
- · ... that can be kernelized to achieve nonlinear models!
 - What is a kernel and how can we apply it at scale?
 Come back on Tuesday and find out!

Key Takeaways

- Distributed PCA
 - Very similar to distributed linear regression:
 - If k is small, simply distribute the storage and computation of X^TX
 - If k is large, use iterative methods (e.g., power iteration) to compute eigenvector-eigenvalue pairs
- Distributed logistic regression
 - Distribute the summands of gradient descent and compute in parallel

Positive Semidefinite Matrices

- For a symmetric matrix $A \in \mathbb{R}^{n \times n}$, the following statements are equivalent:
- 1. *A* is positive semidefinite
- $2. \quad \forall \ x \in \mathbb{R}^n, \ x^T A x \ge 0$
- 3. All eigenvalues of A are greater than or equal to 0
- 4. $\exists U \text{ s.t. } A = U^T U$

Block Matrices

Sometimes, it may be convenient to express a matrix A
as comprised of several smaller matrices:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

• The Schur complement of A_{22} is defined as

$$C = A_{11} - A_{12}A_{22}^{-1}A_{21}$$

 Using the Schur complement, we can succinctly express quantities like

$$\det(A) = \det(A_{22}) * \det(C)$$

$$A^{-1} = \begin{bmatrix} I & 0 \\ -A_{22}^{-1}A_{21} & I \end{bmatrix} \begin{bmatrix} C & 0 \\ 0 & A_{22}^{-1} \end{bmatrix} \begin{bmatrix} I & -A_{12}A_{22}^{-1} \\ 0 & I \end{bmatrix}$$

Orthogonal Matrices

- An orthogonal matrix is a real symmetric matrix whose columns and rows are orthonormal vectors.
- If A is an orthogonal matrix, then this implies that

$$A^T A = A A^T = I$$

or equivalently

$$A^T = A^{-1}$$

Singular Value Decomposition

• Any matrix real $A \in \mathbb{R}^{m \times n}$ can be expressed as the product of three matrices:

$$A = U\Sigma V^T$$

where

- $U \in \mathbb{R}^{m \times m}$ is an orthogonal matrix whose columns are the eigenvectors of AA^T
- $V \in \mathbb{R}^{n \times n}$ is also an orthogonal matrix whose columns are the eigenvectors of A^TA
- $\Sigma \in \mathbb{R}^{m \times n}$ is a diagonal rectangular matrix whose non-zero elements are the square roots of the eigenvalues of AA^T (equivalently, A^TA)