Scalable logistic regression

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Probabilistic classifier

- A logistic regression model is an example of a probabilistic classifier.
- Let $\mathbf{x} \in \mathbb{R}^p$ represents a feature vector and y the target value.
- For a binary classification problem we can use $y \in \{0, 1\}$ or $y \in \{-1, +1\}$.
- We model the relationship between y, and $\mathbf{x}$ using a Bernoulli distribution.

Bernoulli distribution (I)

- A Bernoulli random variable Y is a random variable that can only take two possible values.
- For example, the random variable Y associated to the experiment of tossing a coin.
- Output "heads" is assigned 1 ($Y = 1$), and output "tails" is assigned 0 ($Y = 0$).

Bernoulli distribution (II)

- A Bernoulli distribution is a probability distribution for Y, expressed as

$$p(Y = y) = \text{Ber}(y|\mu) = \begin{cases} \mu & y = 1, \\ 1 - \mu & y = 0, \end{cases}$$

where $\mu = P(Y = 1)$.

- The expression above can be summarized in one line using

$$p(Y = y) = \text{Ber}(y|\mu) = \mu^y (1 - \mu)^{1-y},$$

How are y and **x** related in logistic regression?

- The target feature y follows a Bernoulli distribution

$$p(y|\mathbf{x}) = \text{Ber}(y|\mu(\mathbf{x})).$$

- Notice how the probability $\mu = P(y = 1)$ explicity depends on **x**.

- In logistic regression, the probability $\mu(\mathbf{x})$ is given as

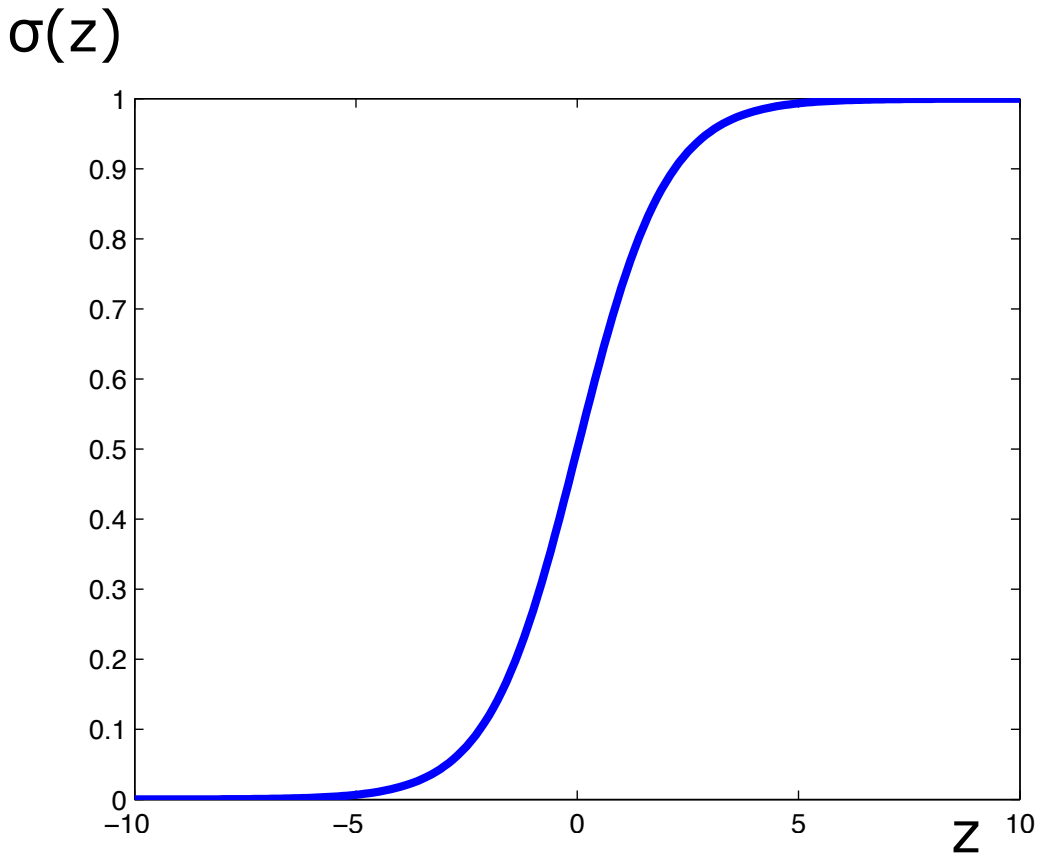
$$\mu(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})} = \sigma(\mathbf{w}^\top \mathbf{x}),$$

where $\sigma(z)$ is known as the *logistic sigmoid* function.

- We then have

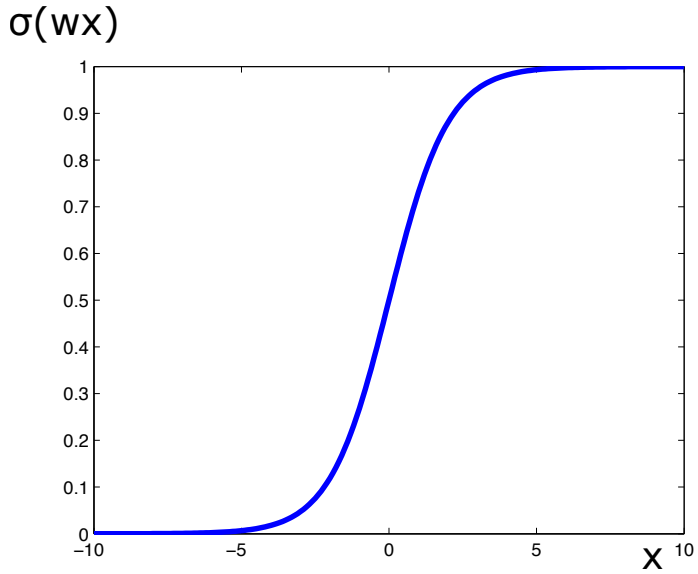
$$p(y|\mathbf{w}, \mathbf{x}) = \text{Ber}(y|\sigma(\mathbf{w}^\top \mathbf{x})).$$

The logistic sigmoid function $\sigma(z)$



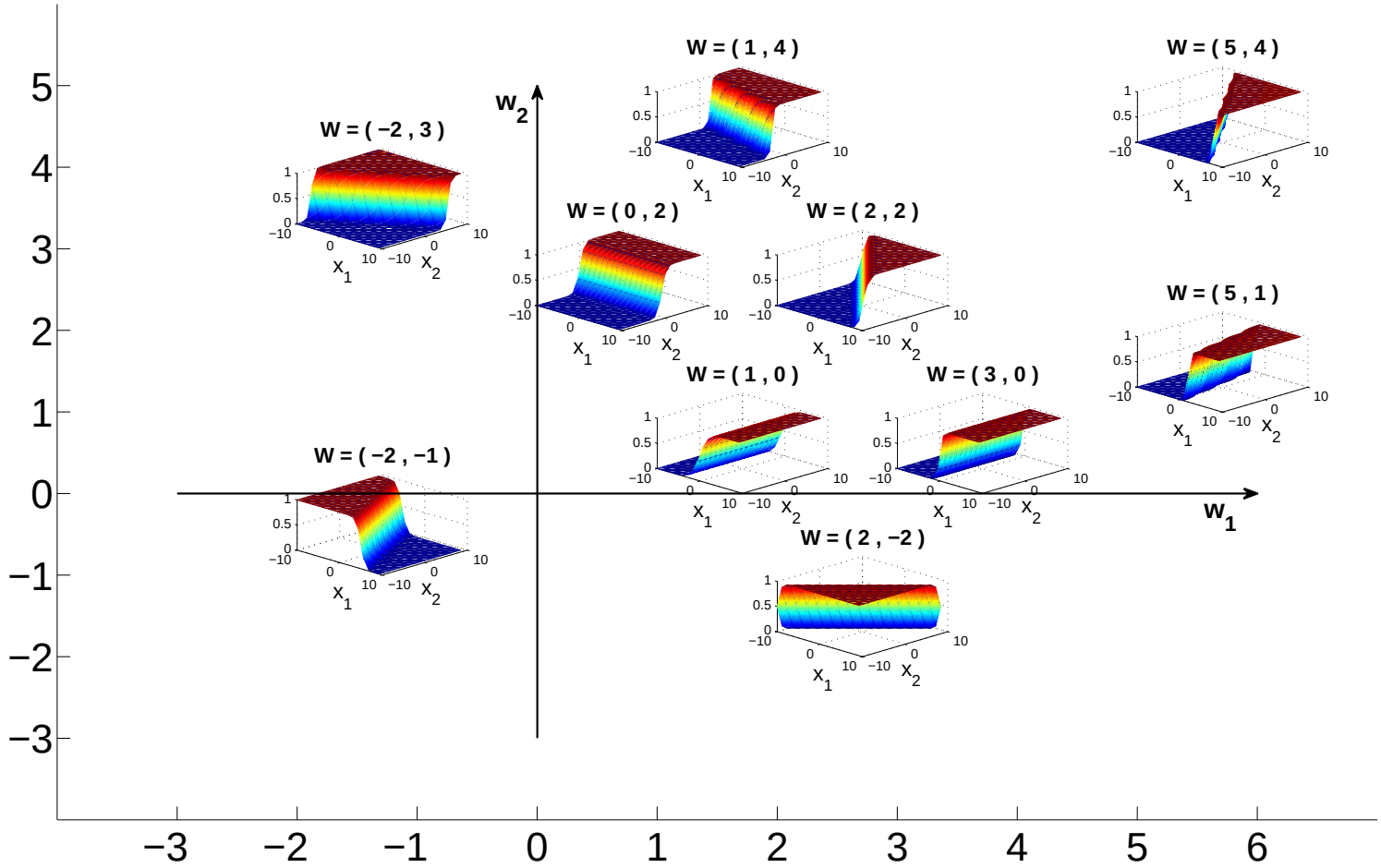
- Recall $\sigma(z) = \dfrac{1}{1 + \exp(-z)}$.
- If $z \to \infty$, $\sigma(z) = 1$. If $z \to -\infty$, $\sigma(z) = 0$. If $z = 0$, $\sigma(z) = 0.5$.

The logistic sigmoid function $\sigma(\mathbf{w}^\top \mathbf{x})$



- We have $z = \mathbf{w}^\top \mathbf{x}$. For simplicity, assume $\mathbf{x} = x$, then $\sigma(wx)$.
- Recall $\sigma(wx) = \dfrac{1}{1 + \exp(-wx)}$.
- So $\left.\dfrac{d\sigma(wx)}{dx}\right|_{x=0} = \dfrac{w}{4}$.

The logistic sigmoid function in 2d



Plot of $\sigma(w_1 x_1 + w_2 x_2)$. Here $\mathbf{w} = [w_1\ w_2]^\top$.

Decision boundary

- After the training phase, we will have an estimator for $\mathbf{w}$.
- For a test input vector $\mathbf{x}_*$, we compute $p(y = 1|\mathbf{w}, \mathbf{x}_*) = \sigma(\mathbf{w}^\top \mathbf{x}_*)$.
- This will give us a value between 0 and 1.
- We define a threshold of 0.5 to decide to which class we assign $\mathbf{x}_*$.
- With this threshold we induce a linear decision boundary in the input space.

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Cross-entropy error function

- Let $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N$.
- We write $\mathbf{X} = [\mathbf{x}_1 \cdots \mathbf{x}_N]^\top$, and $\mathbf{y} = [y_1 \cdots y_N]^\top$.
- Assuming IID observations

$$p(\mathbf{y}|\mathbf{w}, \mathbf{X}) = \prod_{n=1}^{N} p(y_n|\mathbf{w}, \mathbf{x}_n) = \prod_{n=1}^{N} \mathrm{Ber}(y_n|\sigma(\mathbf{w}^\top \mathbf{x}_n)).$$

- The cross-entropy function or negative log-likelihood is given as

$$\begin{aligned} NLL(\mathbf{w}) &= -\log p(\mathbf{y}|\mathbf{w}, \mathbf{X}) \\ &= -\sum_{n=1}^{N} \{y_n \log[\sigma(\mathbf{w}^\top \mathbf{x}_n)] + (1 - y_n) \log[1 - \sigma(\mathbf{w}^\top \mathbf{x}_n)]\}, \end{aligned}$$

which can be minimised with respect to $\mathbf{w}$.

Gradient and Hessian of $NLL(\mathbf{w})$

- It can be shown that the gradient $\mathbf{g}(\mathbf{w})$ of $NLL(\mathbf{w})$ is given as

$$\mathbf{g}(\mathbf{w}) = \frac{d}{d\mathbf{w}} NLL(\mathbf{w}) = \sum_{n=1}^{N} [\sigma(\mathbf{w}^\top \mathbf{x}_n) - y_n]\mathbf{x}_n = \mathbf{X}^\top(\boldsymbol{\sigma} - \mathbf{y}),$$

where $\boldsymbol{\sigma} = [\sigma(\mathbf{w}^\top \mathbf{x}_1) \cdots \sigma(\mathbf{w}^\top \mathbf{x}_N)]^\top$.

- It can also be shown that the Hessian $\mathbf{H}(\mathbf{w})$ of $NLL(\mathbf{w})$ is given as

$$\mathbf{H}(\mathbf{w}) = \frac{d}{d\mathbf{w}} \mathbf{g}(\mathbf{w})^\top = \sum_{n=1}^{N} \sigma(\mathbf{w}^\top \mathbf{x}_n)[1 - \sigma(\mathbf{w}^\top \mathbf{x}_n)]\mathbf{x}_n \mathbf{x}_n^\top = \mathbf{X}^\top \Sigma \mathbf{X},$$

where $\Sigma = \text{diag}([\sigma(\mathbf{w}^\top \mathbf{x}_1)[1 - \sigma(\mathbf{w}^\top \mathbf{x}_1)], \cdots, \sigma(\mathbf{w}^\top \mathbf{x}_N)[1 - \sigma(\mathbf{w}^\top \mathbf{x}_N)]])$.

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General problem

- We are given a function $f(\mathbf{w})$, where $\mathbf{w} \in \mathbb{R}^p$.
- Aim: to find a value for $\mathbf{w}$ that minimises $f(\mathbf{w})$.
- Use an iterative procedure

$$\mathbf{w}_{k+1} = \mathbf{w}_k + \eta \mathbf{d}_k,$$

where $\mathbf{d}_k$ is known as the search direction and it is such that

$$f(\mathbf{w}_{k+1}) < f(\mathbf{w}_k).$$

- The parameter η is known as the **step size** or **learning rate**.

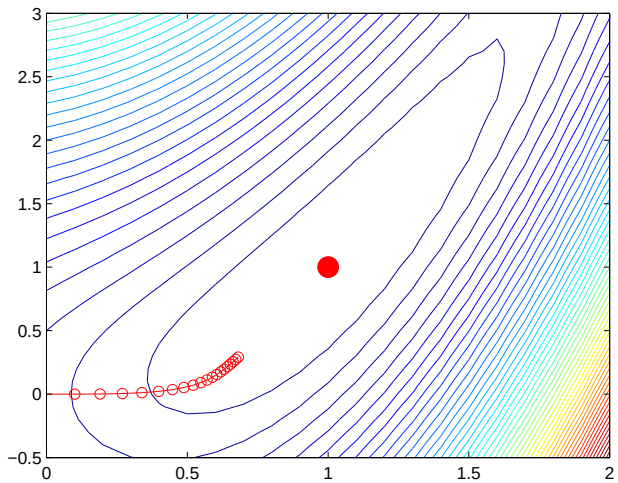
Gradient descent

- Perhaps, the simplest algorithm for unconstrained optimisation.
- It assumes that $\mathbf{d}_k = -\mathbf{g}_k$, where $\mathbf{g}_k = \mathbf{g}(\mathbf{w}_k)$.
- Also known as **steepest descent**.
- It can be written like

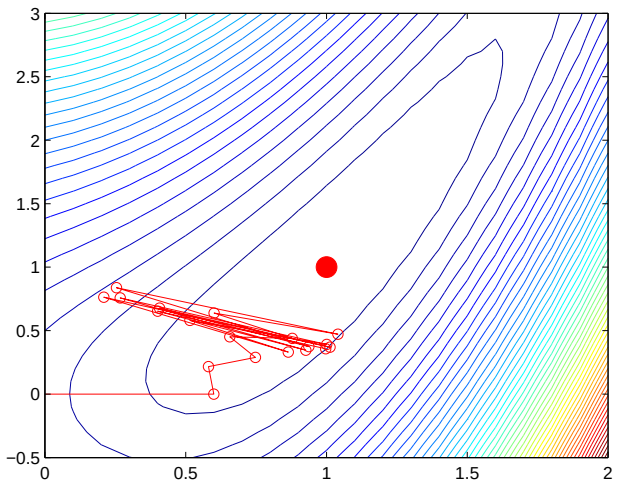
$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta \mathbf{g}_k.$$

Step size

- The main issue in gradient descent is how to set the step size.
- If it is too small, convergence will be very slow. If it is too large, the method can fail to converge at all.



(a)



(b)

The function to optimise is $f(w_1, w_2) = 0.5(w_1^2 - w_2)^2 + 0.5(w_1 - 1)^2$. The minimum is at $(1, 1)$. In (a) $\eta = 0.1$. In (b) $\eta = 0.6$.

Alternatives to choose the step size η

- Line search methods (there are different alternatives).
- Line search methods may use search directions other than the steepest descent direction.
- Conjugate gradient (method of choice for quadratic objectives $f(\mathbf{w}) = \mathbf{w}^\top \mathbf{A}\mathbf{w}$).

Newton's method (I)

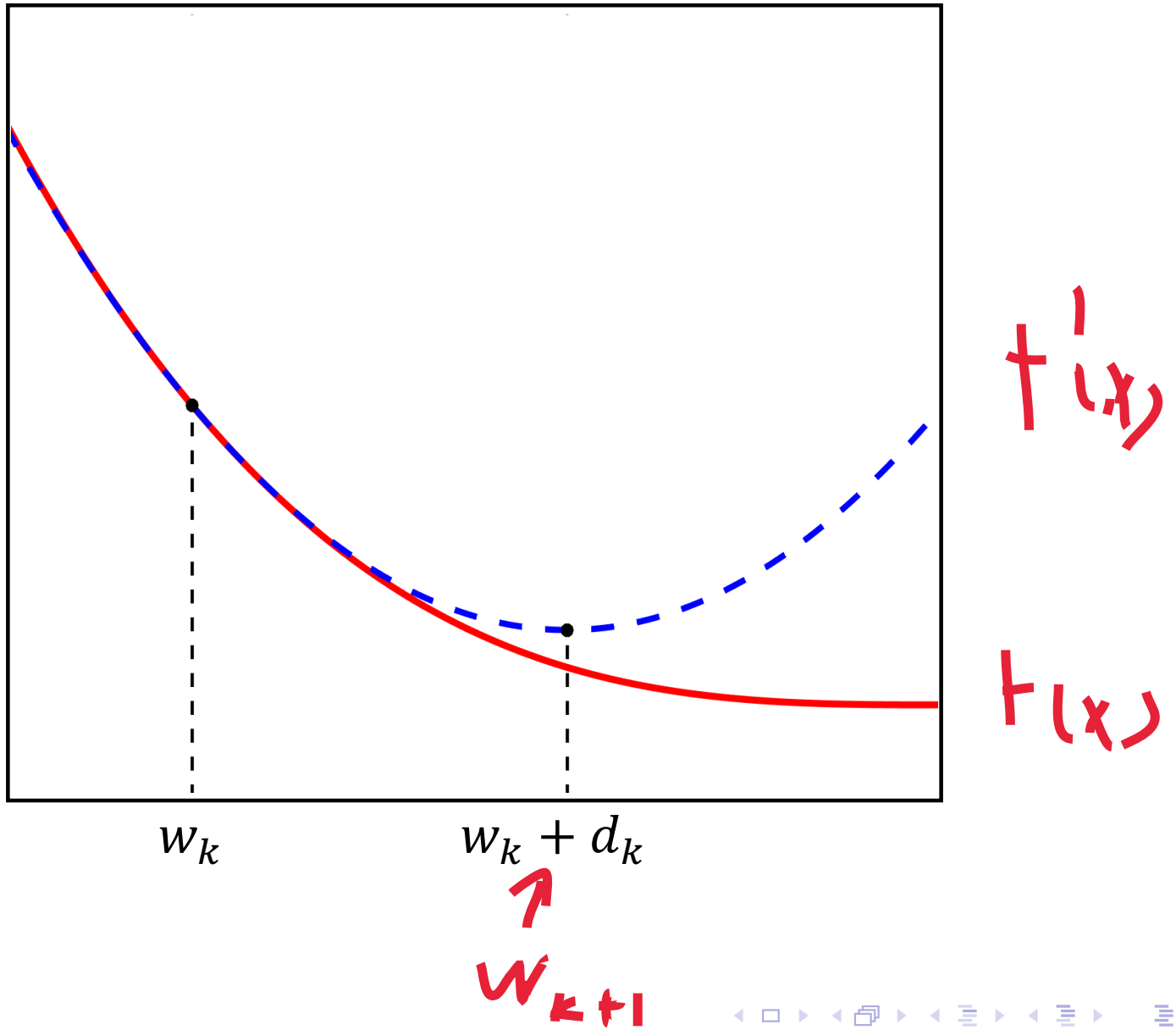
- Another important search direction is the *Newton* direction.
- It derives a faster optimisation algorithm by taking the curvature of the space (i.e., the Hessian) into account.
- Optimisation methods that include the Hessian are also known as second order optimisation methods.
- In Newton's algorithm

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta \mathbf{H}_k^{-1} \mathbf{g}_k,$$

where $\mathbf{g}_k = \mathbf{g}(\mathbf{w}_k)$, and $\mathbf{H}_k = \mathbf{H}(\mathbf{w}_k)$.

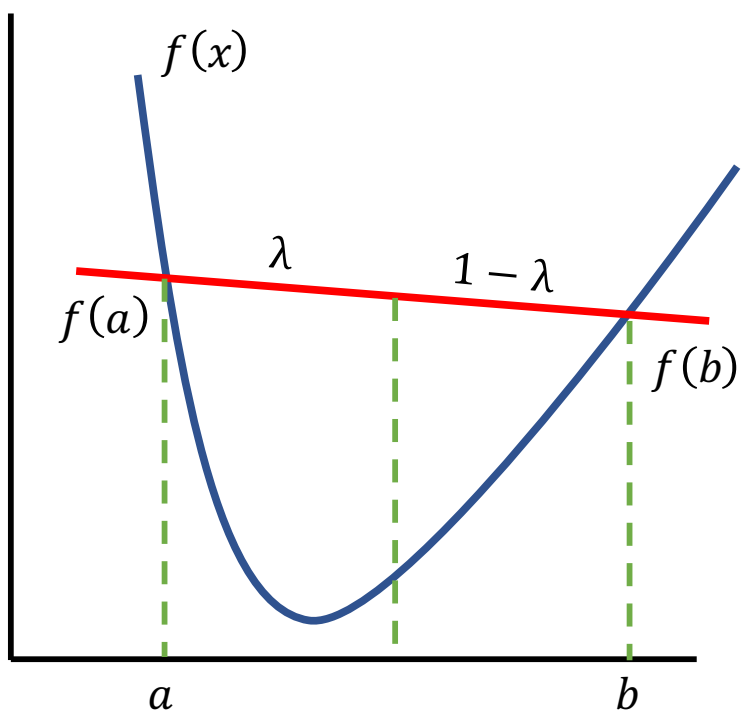
- Usually $\eta = 1$, and $\mathbf{d}_k = -\mathbf{H}_k^{-1} \mathbf{g}_k$.

Newton's method (II)

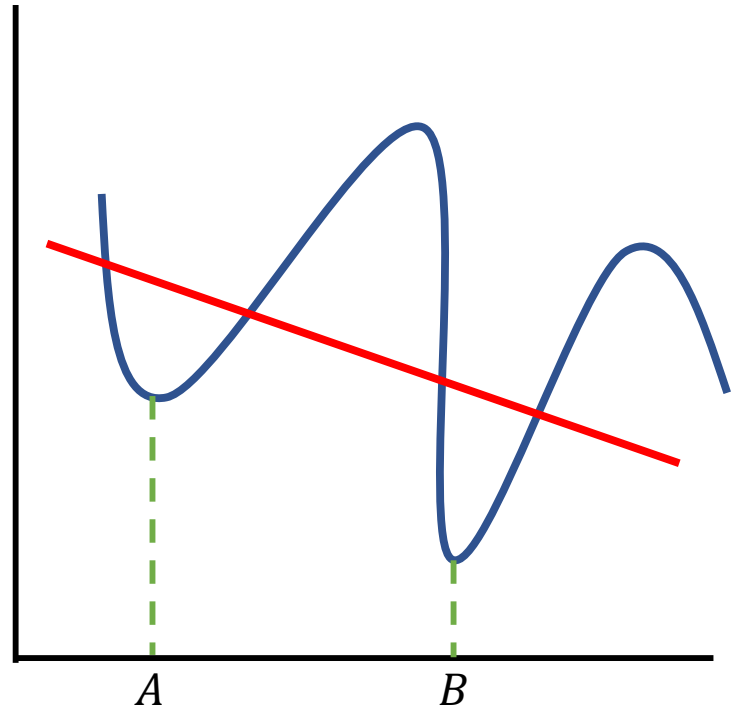


Newton's method and convex functions (I)

- Newton's method requires that $\mathbf{H}_k$ be positive definite (p.d.)
- The condition holds if the function is strictly convex.



(a)



(b)

In (a), an illustration of a convex function. The chord joining $(a, f(a))$ and $(b, f(b))$ lies above the function. In (b), a function that is neither convex nor concave.

Newton's method and convex functions (II)

- If not strictly convex, $\mathbf{H}_k$ may not be p.d., and $\mathbf{d}_k = -\mathbf{H}_k^{-1}\mathbf{g}_k$ may not be a descent direction.

- Alternatives:
  - If $\mathbf{H}_k$ is not positive definite, use $\mathbf{d}_k = -\mathbf{g}_k$ instead.
  - Use the *Levenberg Marquardt* algorithm, which compromises between the Newton direction and the steepest direction.
  - Rather than computing $\mathbf{d}_k = -\mathbf{H}_k^{-1}\mathbf{g}_k$, find $\mathbf{d}_k$ that solves the linear system $\mathbf{H}_k\mathbf{d}_k = -\mathbf{g}_k$ using an iterative procedure. Stop when needed (**truncated Newton**).

Quasi-Newton methods

- The main drawback of the Newton direction is the need for the Hessian.
- Explicit computation of this matrix of second derivatives can sometimes be a cumbersome, error-prone, and expensive process.
- Quasi-Newton search directions provide an attractive alternative to Newton's method.
- They do not require computation of the Hessian and yet still attain a faster rate of convergence.
- In place of the true Hessian $\mathbf{H}_k$, they use an approximation $\mathbf{B}_k$, which is updated after each step to take account of the additional knowledge gained during the step.

BFGS formula for $\mathbf{H}_k$

- In the Broyden, Fletcher, Goldfarb, and Shanno (BFGS) formula

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{\mathbf{z}_k \mathbf{z}_k^\top}{\mathbf{z}_k^\top \mathbf{s}_k} - \frac{(\mathbf{B}_k \mathbf{s}_k)(\mathbf{B}_k \mathbf{s}_k)^\top}{\mathbf{s}_k^\top \mathbf{B}_k \mathbf{s}_k},$$

  where $\mathbf{s}_k = \mathbf{w}_k - \mathbf{w}_{k-1}$ and $\mathbf{z}_k = \mathbf{g}_k - \mathbf{g}_{k-1}$.

- This is a rank-two update to the matrix, and ensures that the matrix remains positive definite.

- Ussually $\mathbf{B}_0 = \mathbf{I}$.

- The search direction is then $\mathbf{d}_k = -\mathbf{B}_k^{-1} \mathbf{g}_k$.

BFGS formula for $\mathbf{H}_k^{-1}$

- BFGS can alternatively update $\mathbf{C}_k = \mathbf{H}_k^{-1}$ using

$$\mathbf{C}_{k+1} = \left(\mathbf{I} - \frac{\mathbf{s}_k \mathbf{z}_k^\top}{\mathbf{z}_k^\top \mathbf{s}_k}\right) \mathbf{C}_k \left(\mathbf{I} - \frac{\mathbf{z}_k \mathbf{s}_k^\top}{\mathbf{z}_k^\top \mathbf{s}_k}\right) + \frac{\mathbf{s}_k \mathbf{s}_k^\top}{\mathbf{z}_k^\top \mathbf{s}_k}.$$

- The search direction is then $\mathbf{d}_k = -\mathbf{C}_k \mathbf{g}_k$.

Limited memory BFGS (L-BFGS)

- Since storing the Hessian takes $O(p^2)$ space, for very large problems, one can use limited memory BFGS, or L-BFGS.
- In L-BFGS, $\mathbf{H}_k$ or $\mathbf{H}_k^{-1}$ is approximated by a diagonal plus low rank matrix.
- In particular, the product $\mathbf{B}_k^{-1}\mathbf{g}_k$ can be obtained by performing a sequence of inner products with $\mathbf{s}_k$ and $\mathbf{z}_k$, using only the m most recent $(\mathbf{s}_k, \mathbf{z}_k)$ pairs, and ignoring older information.
- The storage requirements are therefore $O(mp)$. Typically $m \sim 20$ suffices for good performance.

Optimisation methods applied to logistic regression

All the methods described above can be applied to find the parameter vector $\mathbf{w}$ that minimises the negative log-likelihood $NLL(\mathbf{w})$ in logistic regression.

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Algorithms in summation form

- When an algorithm sums over the data, we can easily distribute the calculations over multiple workers (e.g. cores).
- We just divide the dataset into as many pieces as there are workers, give each worker its share of the data to sum the equations over, and aggregate the result at the end.
- Both the gradient and Hessian in the optimisation algorithms we saw before have a summation form.
- Notice that the summation form does not change the underlying algorithm: it is not an approximation but an exact implementation.

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Stochastic gradient descent (I)

- Traiditionally in machine learning, the gradient $\mathbf{g}_k$ and the Hessian $\mathbf{H}_k$ are computed using the whole dataset $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N$.
- There are settings, though, where only a subset of the data can be used.
- **Online learning**: the instances $(\mathbf{x}_n, y_n)$ appear one at a time.
- **Large datasets**: computing the exact values for $\mathbf{g}_k$ and $\mathbf{H}_k$ would be expensive, if not impossible.

Stochastic gradient descent (II)

- In stochastic gradient descent (SGD), the gradient $\mathbf{g}_k$ is computed using a subset of the instances available.
- The word stochastic refers to the fact that the value for $\mathbf{g}_k$ will depend on the subset of the instances chosen for computation.

Stochastic gradient descent (III)

- In the stochastic setting, a better estimate can be found if the gradient is computed using

$$\mathbf{g}_k = \frac{1}{|S|} \sum_{i \in S} \mathbf{g}_{k,i},$$

where $S \in \mathcal{D}$, $|S|$ is the cardinality of S, and $\mathbf{g}_{k,i}$ is the gradient at iteration k computed using the instance $(\mathbf{x}_i, y_i)$.

- This setting is called Mini-batch gradient descent.

- For logistic regression, $\mathbf{g}_{k,i}$ would be the gradient computed for $-\log p(y_i|\mathbf{w}, \mathbf{x}_i)$.

Step size in SGD

- Choosing the value of η is particularly important in SGD since there is no easy way to compute it.
- Usually the value of η will depend on the iteration k, η_k.
- It should follow the **Robbins-Monro** conditions

$$\sum_{k=1}^{\infty} \eta_k = \infty, \quad \sum_{k=1}^{\infty} \eta_k^2 < \infty.$$

- Various formulas for η_k can be used

$$\eta_k = \frac{1}{k}, \quad \eta_k = \frac{1}{(\tau_0 + k)^{\kappa}},$$

where τ_0 slows down early interations and $\kappa \in (0.5, 1]$.

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What is regularisation?

- It refers to a technique used for preventing overfitting in a predictive model.
- It consists in adding a term (a regulariser) to the objective function that encourages simpler solutions.

- With regularisation, the objective function for logistic regression would be

$$f(\mathbf{w}) = NLL(\mathbf{w}) + \lambda R(\mathbf{w}),$$

where $R(\mathbf{w})$ is the regularisation term and λ the regularisation parameter.

- If $\lambda = 0$, we get $f(\mathbf{w}) = NLL(\mathbf{w})$.

Different types of regularisation

- The objective function for logistic regression would be

$$f(\mathbf{w}) = NLL(\mathbf{w}) + \lambda R(\mathbf{w}),$$

where $R(\mathbf{w})$ follows as

$$R(\mathbf{w}) = \alpha \|\mathbf{w}\|_1 + (1-\alpha)\frac{1}{2}\|\mathbf{w}\|_2^2,$$

where $\|\mathbf{w}\|_1 = \sum_{m=1}^{p} |w_m|$, and $\|\mathbf{w}\|_2^2 = \sum_{m=1}^{p} w_m^2$.

- If $\alpha = 1$, we get ℓ_1 regularisation.
- If $\alpha = 0$, we get ℓ_2 regularisation.
- If $0 < \alpha < 1$, we get the elastic net regularisation.
- In Spark, λ is `regParam` and α is `elasticNetParam`.

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Binary logistic regression for multi-class problems

- The implementation of multi-class logistic regression for K classes in Spark uses $K - 1$ binary logistic regression models.

- The idea is to choose one class as a "pivot" and train $K - 1$ binary logistic regression models between the pivot class and any of the other classes.

A pivot class

- In `spark.ml` the pivot class is the class "0", and the probabilities for each class are given as

$$p(y = 0|\mathbf{x}, \mathbf{w}) = \frac{1}{1 + \sum_{\ell=1}^{K-1} \exp(\mathbf{w}_\ell^\top \mathbf{x})}$$

$$p(y = k|\mathbf{x}, \mathbf{w}) = \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{1 + \sum_{\ell=1}^{K-1} \exp(\mathbf{w}_\ell^\top \mathbf{x})}, \quad k = 1, \ldots, K-1$$

- Given a dataset, it is possible to write an expression for the negative log-likelihood and then minimise it using any of the methods based on the gradient or the gradient and the Hessian.

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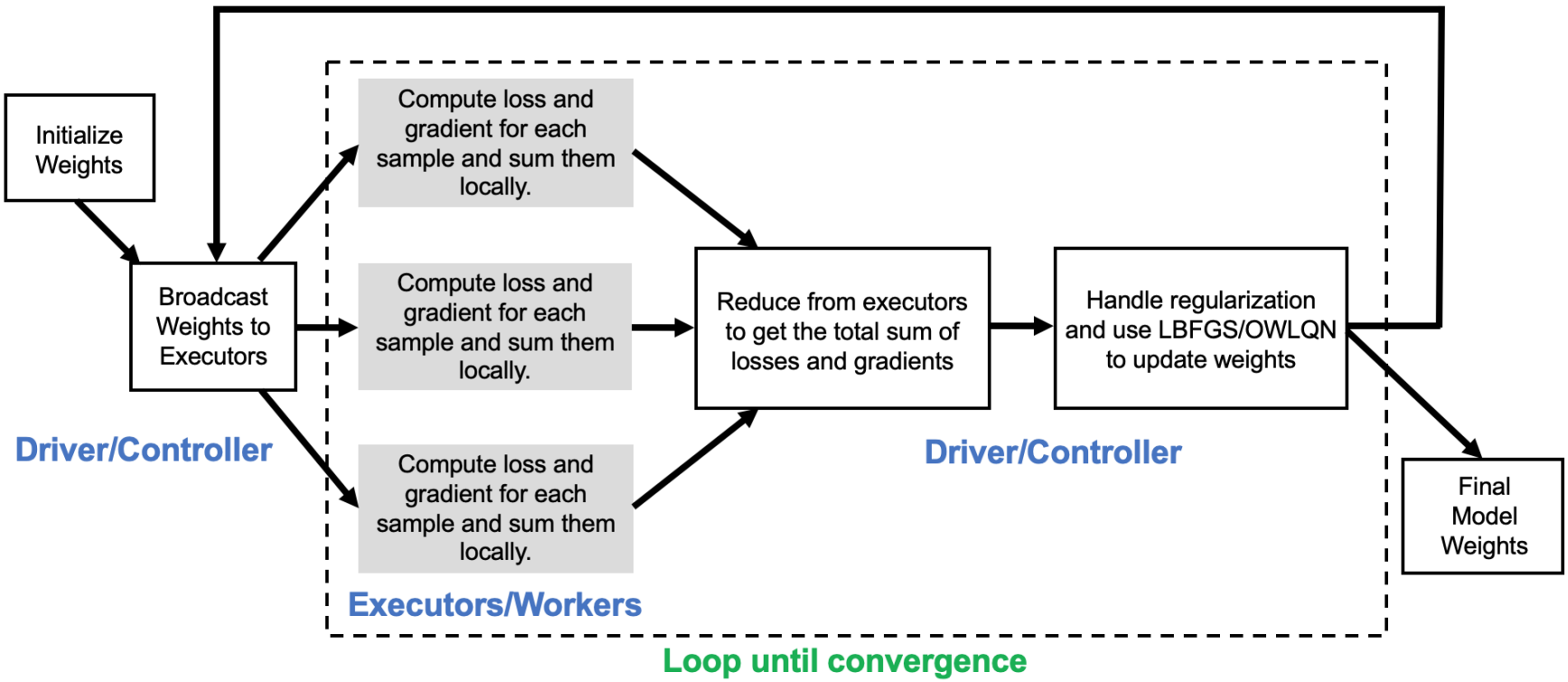
Update of **w** in Apache Spark



`LogisticRegression()`

- `LogisticRegression()` works with DataFrames.
- It is possible to use regularisation ℓ_1, ℓ_2 or Elastic Net.
- L-BFGS is used as a solver for `LogisticRegression()`, with ℓ_2.
- When ℓ_1, or Elastic Net are used, a variant of L-BFGS, known as Orthant-Wise Limited-memory Quasi-Newton (OWL-QN) is used instead.

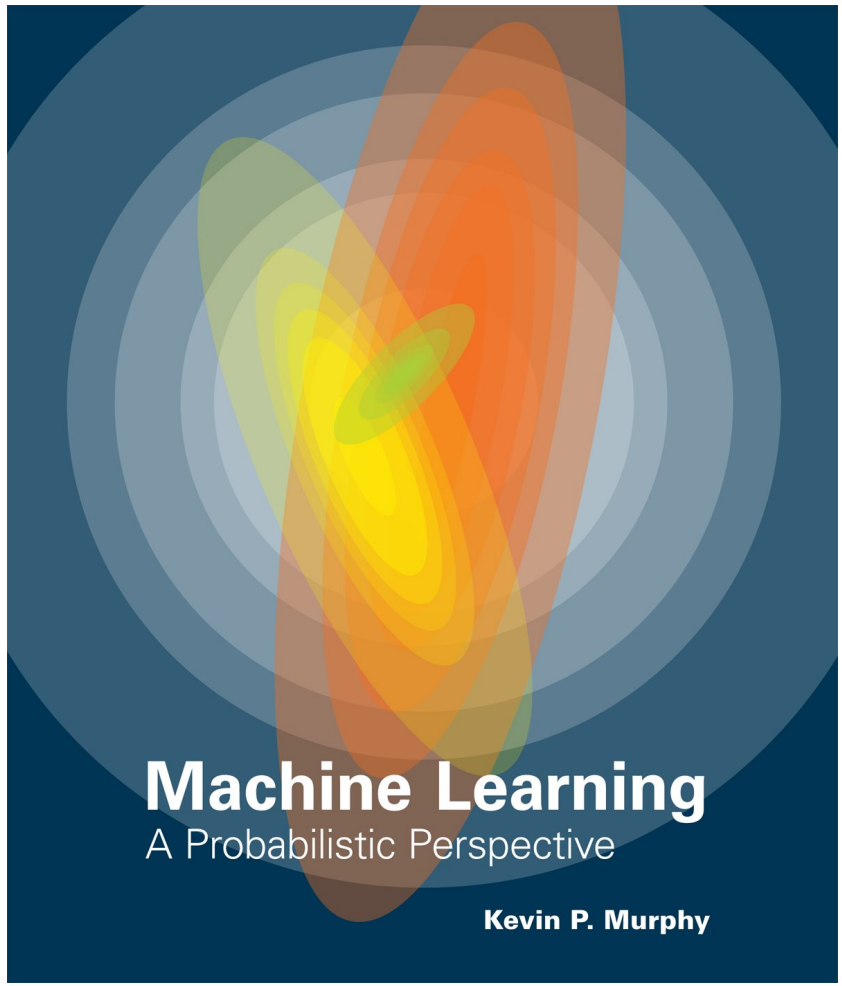
Parameters to adjust

- **`maxIter`**: max number of iterations.
- **`regParam`**: regularization parameter (≥ 0).
- **`elasticNetParam`**: the ElasticNet mixing parameter, in range $[0, 1]$. For $\alpha = 0$, the penalty is an ℓ_2 penalty. For $\alpha = 1$, it is an ℓ_1 penalty.
- **`family`**: the name of family which is a description of the label distribution to be used in the model. Supported options: auto, binomial, multinomial.
- **`standardization`**: whether to standardize the training features before fitting the model. It can be true or false.

Contents

References used in this lecture

Book: *Machine Learning: A Probabilistic Perspective* by Kevin P Murphy, 2012.



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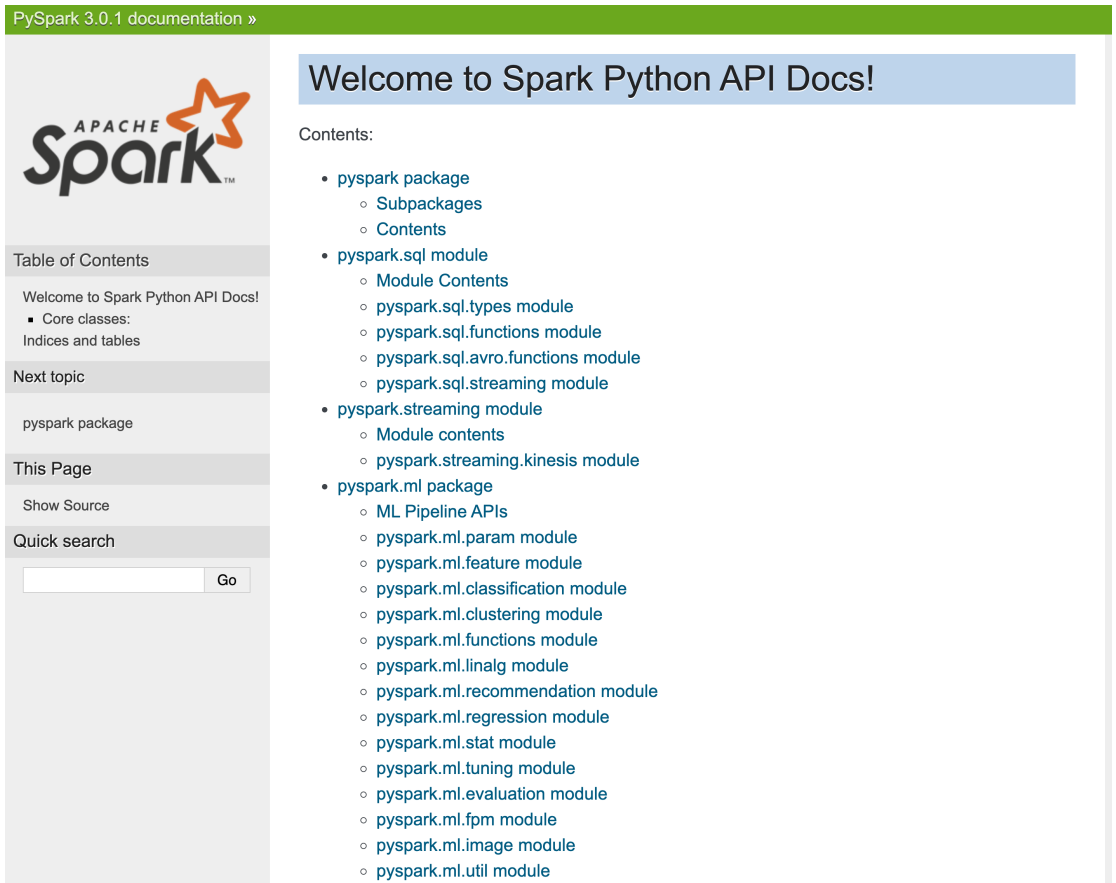

`https://spark.apache.org/docs/3.0.1/api/python/index`

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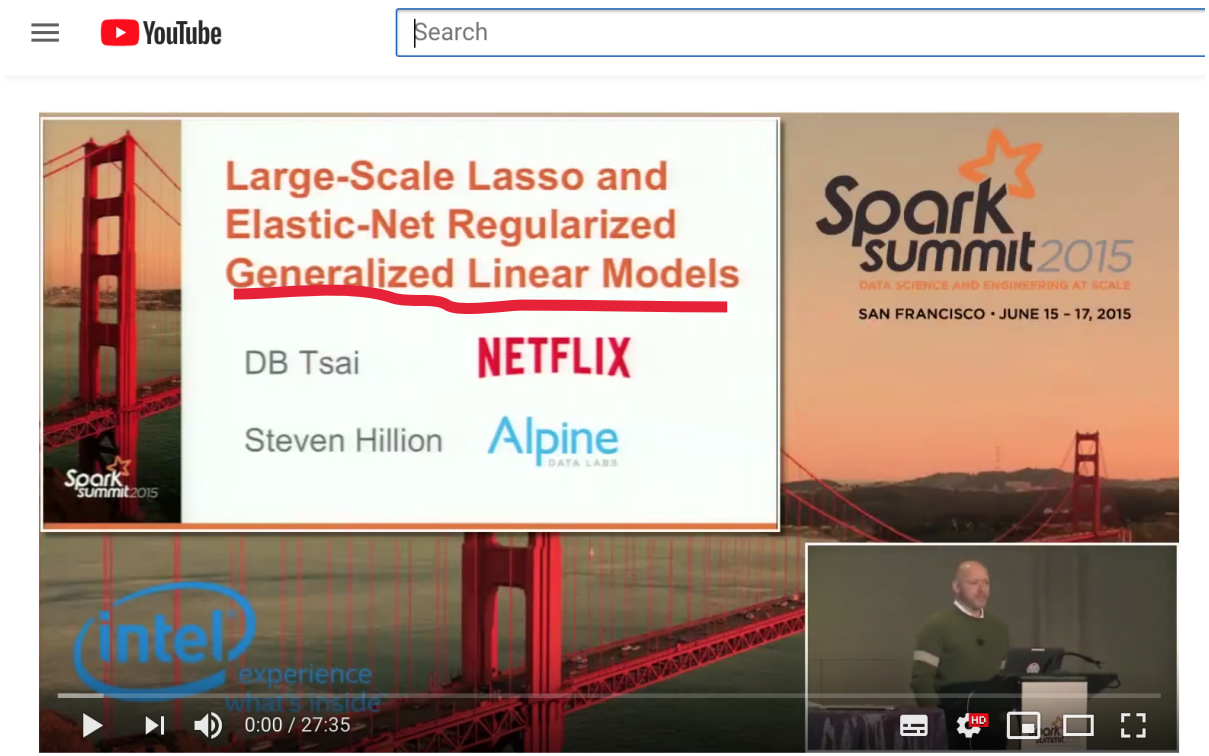
Youtube video: *Large-Scale Lasso and Elastic-Net Regularized Generalized Linear Models* by DB Tsai (from Netflix) and Steven Hillion (from Alpine Data Labs).



2015-06-15 Large-Scale Elastic-Net Regularized Generalized Linear Models at Spark Summit 2015

`https://www.youtube.com/watch?v=TJer4ibUZ0I`

References used in this lecture

Paper: *Map-Reduce for Machine Learning on Multicore* by C-T Chu et al. (2007).

Map-Reduce for Machine Learning on Multicore

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Abstract

We are at the beginning of the multicore era. Computers will have increasingly many cores (processors), but there is still no good programming framework for these architectures, and thus no simple and unified way for machine learning to take advantage of the potential speed up. In this paper, we develop a broadly applicable parallel programming method, one that is easily applied to *many* different learning algorithms. Our work is in distinct contrast to the tradition in machine learning of designing (often ingenious) ways to speed up a *single* algorithm at a time. Specifically, we show that algorithms that fit the Statistical Query model [15] can be written in a certain "summation form," which allows them to be easily parallelized on multicore computers. We adapt Google's map-reduce [7] paradigm to demonstrate this parallel speed up technique on a variety of learning algorithms including locally weighted linear regression (LWLR), k-means, logistic regression (LR), naive Bayes (NB), SVM, ICA, PCA, gaussian discriminant analysis (GDA), EM, and backpropagation (NN). Our experimental results show basically linear speedup with an increasing number of processors.

References used in this lecture

Paper: *Optimization Methods for Large Scale Machine Learning* by L. Bottou et al. (2018).

Optimization Methods for Large-Scale Machine Learning

Léon Bottou* Frank E. Curtis† Jorge Nocedal‡

February 12, 2018

Abstract

This paper provides a review and commentary on the past, present, and future of numerical optimization algorithms in the context of machine learning applications. Through case studies on text classification and the training of deep neural networks, we discuss how optimization problems arise in machine learning and what makes them challenging. A major theme of our study is that large-scale machine learning represents a distinctive setting in which the stochastic gradient (SG) method has traditionally played a central role while conventional gradient-based nonlinear optimization techniques typically falter. Based on this viewpoint, we present a comprehensive theory of a straightforward, yet versatile SG algorithm, discuss its practical behavior, and highlight opportunities for designing algorithms with improved performance. This leads to a discussion about the next generation of optimization methods for large-scale machine learning, including an investigation of two main streams of research on techniques that diminish noise in the stochastic directions and methods that make use of second-order derivative approximations.