Large-Scale Optimization

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EECS-6898, Columbia University - Fall, 2010

Learning and Optimization

In most cases, learning from data reduces to optimizing a function with respect to model parameters

Given training data $D = \{x_i, y_i\}_{i=1,\dots,n}$ we want to learn a model

prediction $y = f(x; w)$ $\qquad$ $e.g., x \in \Re^d, y \in \Re$ or $y \in \{-1, 1\}$

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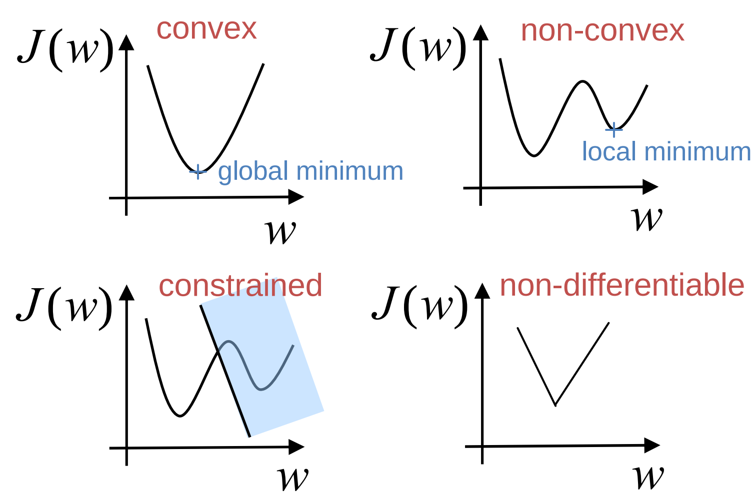
- Convex vs non-convex
- Constrained vs unconstrained
- Smooth vs non-differentiable

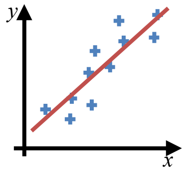
twice differentiable



Examples

Linear regression $y = w^T x + w_0$ $\quad x \in \Re^d, y \in \Re$

Absorb w_0 in w by adding
a dummy variable in x: $x_0 = 1$



$$J(w) = \sum_i (w^T x_i - y_i)^2 + \lambda w^T w$$

convex, smooth, unconstrained

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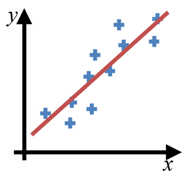

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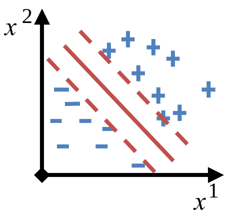
Linear SVM $y = \mathrm{sgn}(w^T x + w_0)$ $x \in \Re^d, y \in \{-1, 1\}$



$$J(w) = \sum_i \max(0, 1 - y_i w^T x_i) + \lambda w^T w$$

convex, non-differentiable, unconstrained

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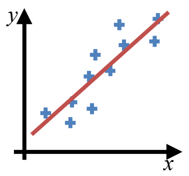

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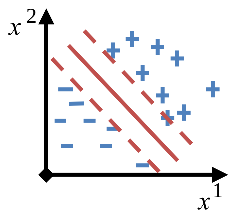

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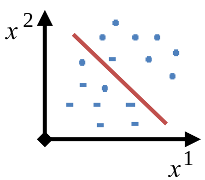
Logistic Regression $p(y=1 \mid x) = \sigma(w^T x + w_0)$ $x \in \Re^d, y \in \{-1, 1\}$

$\sigma(x) = 1/(1+e^{-x})$ probabilistic



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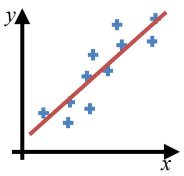

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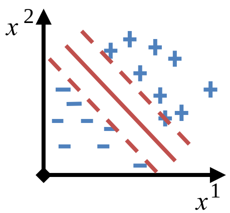

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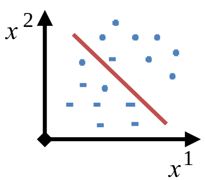

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Nonlinear (kernelized) versions: replace $w^T x$ with $\sum_i w^i k(x, x_i)$

- 2-norm regularizer changes to $w^T K w$ where K is the kernel matrix
- Same properties of the functions as their linear versions

Popular Optimization Methods

First Order Methods

- Use gradient of the function to iteratively find the local minimum
- Easy to compute and run but slow convergence
- Gradient (steepest) descent
- Coordinate descent
- Conjugate Gradient
- Stochastic Gradient Descent

Second Order Methods

- Use gradients and Hessian (curvature) iteratively
- Computationally more demanding but fast convergence
- Newton's method
- Quasi-Newton methods (BFGS and variants)
- Stochastic Quasi-Newton methods

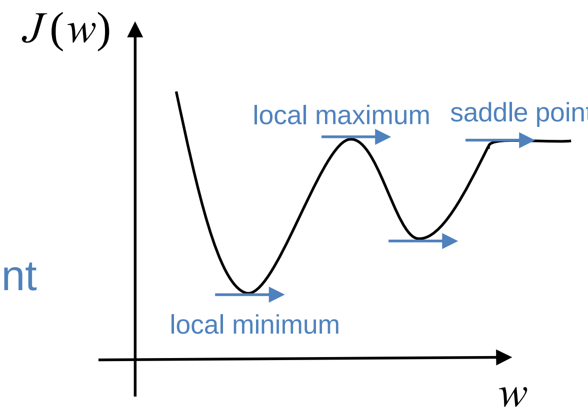
Other than line-search based methods: Trust-region

Conditions for Local Minimum

- If $\hat{w}$ is a local-minimizer then,
  - First-order necessary condition

Gradient $$\frac{\partial J(w)}{\partial w} = \nabla J(\hat{w}) = 0$$

stationary point



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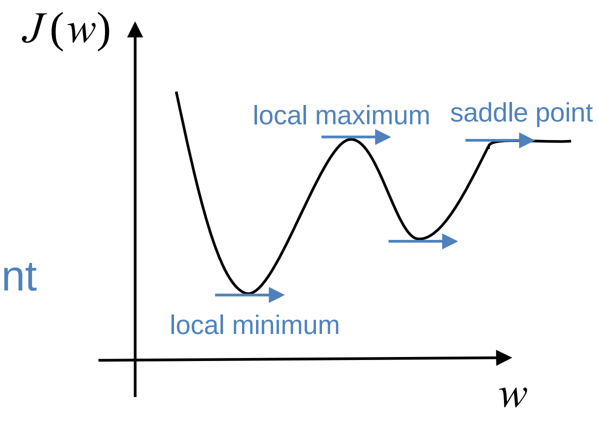

  - Second-order necessary condition

Hessian $$\frac{\partial^2 J(w)}{\partial w \partial w^T} = \nabla^2 J(\hat{w}) \text{ is PSD}$$

positive semi-definite

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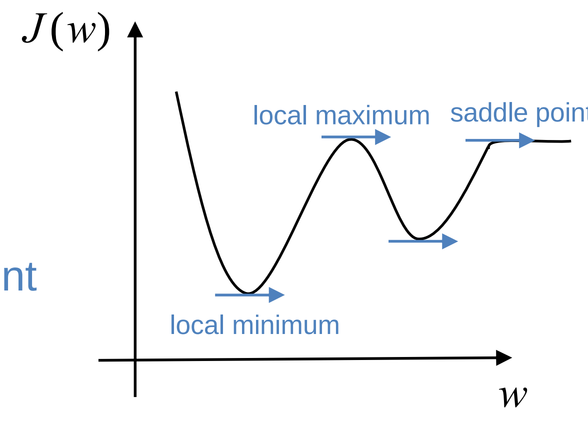

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  - Sufficient conditions

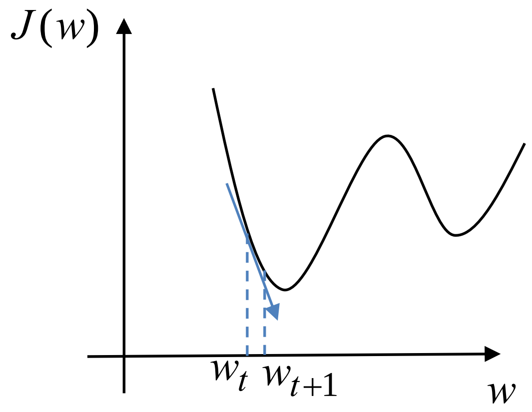
$$\nabla J(\hat{w}) = 0 \text{ and } \nabla^2 J(\hat{w}) \text{ is PD}$$ positive definite (strictly PD)

For smooth convex function → any stationary point is a global minimizer

Gradient Descent

Iteratively estimates new parameter values

$$w_{t+1} = w_t - \eta_t \nabla J(w_t)$$



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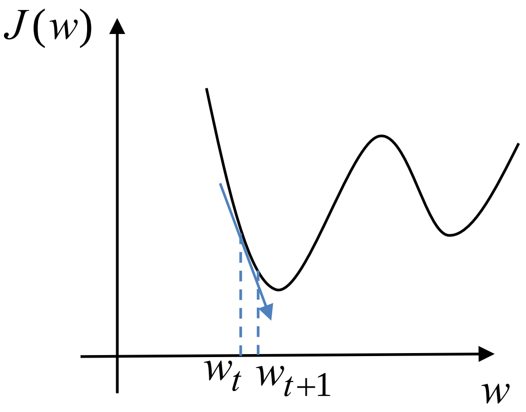

But this is not sufficient to reach local minima !

One has to make sure $\nabla J(w_t) \rightarrow 0$

Step-length must satisfy the Wolfe conditions of sufficient decrease

search direction

$$J(w_t + \eta_t p_t) \leq J(w_t) + c_1 \eta_t \nabla J(w_t) p_t \qquad 0 < c_1 < 1$$

Gradient descent converges to local minimum if step size is sufficiently small !

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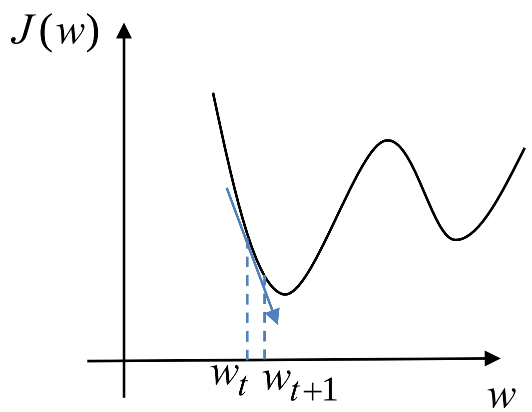

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Gradient descent converges to local minimum if step size is sufficiently small !

Rate of Convergence: Linear

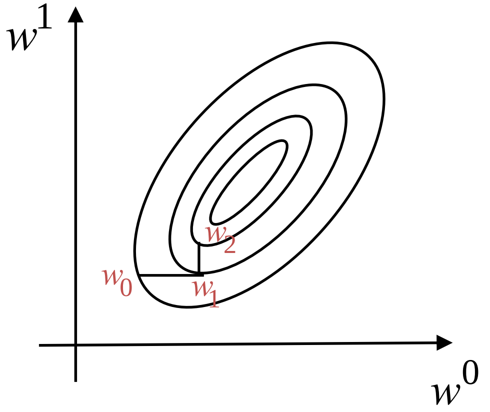
$$\frac{\|w_{t+1} - \hat{w}\|}{\|w_t - \hat{w}\|} \leq r$$

Painfully slow in practice, many heuristics are used (e.g., momentum)

Coordinate Descent

Updates one coordinate at a time keeping others fixed

$$w_{t+1}^{i} = w_{t}^{i} - \eta_t \nabla J(w_t^i)$$



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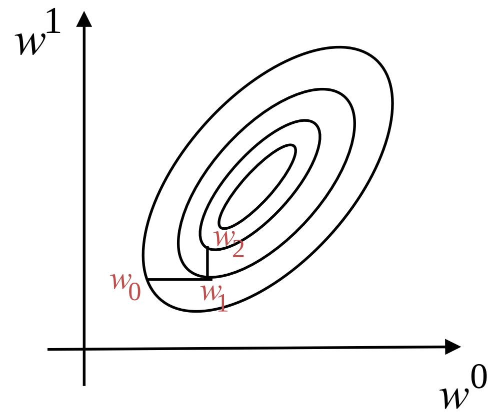

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Properties

- Very simple and easy to implement – reasonable when variables are loosely coupled
- Can be inefficient in practice (may take long time to converge)
- Convergence not guaranteed, in general

Block Coordinate Descent

- Update a small set of coordinates simultaneously
- Has been used successfully for training large SVMs

Conjugate Gradient

Parameters are searched along conjugate directions

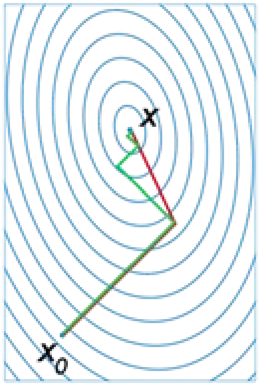
Conjugacy: Two vectors p_1 and p_2 are conjugate wrt H if

$$p_1^T H p_2 = 0$$

Starting with $p_0 = -\nabla J(w_0)$

$$w_{t+1} = w_t + \alpha_t p_t$$

green: GD
red: CG



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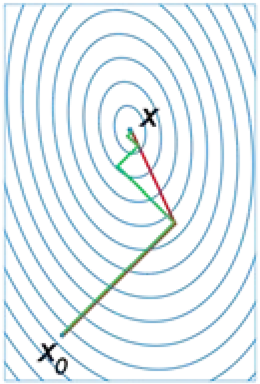

Starting with $p_0 = -\nabla J(w_0)$

$$\boxed{w_{t+1} = w_t + \alpha_t p_t}$$

Successive conjugate directions as linear combination of gradient direction and previous conjugate direction

$$p_t = -\nabla J(w_t) + \beta_t p_{t-1} \qquad t = 1,2,\ldots.$$

Exact $\alpha_t = \dfrac{\nabla J(w_t)^T p_t}{p_t^T H_t p_t}$

But usually picked something that satisfies Wolfe's conditions !

$$\beta_t = \frac{\nabla J(w_t)^T (\nabla J(w_t) - \nabla J(w_{t-1}))}{p_{t-1}^T (\nabla J(w_t) - \nabla J(w_{t-1}))}$$

Hestenes-Stiefel form

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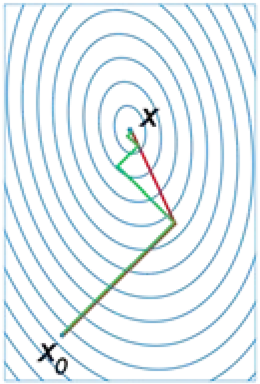

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Hestenes-Stiefel form

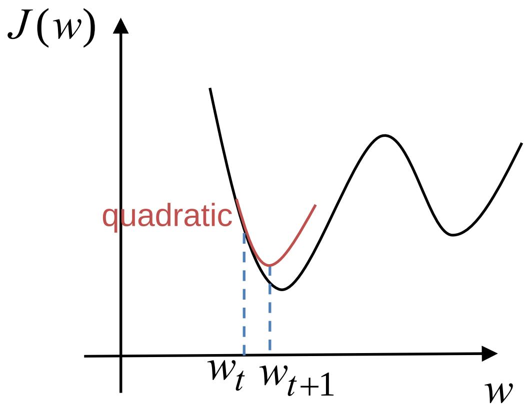
Properties

- For quadratic functions, guaranteed to return the optimal in at most d iterations
- Use preconditioning to increase the convergence rate: make condition number of Hessian as small as possible

Newton's Method

Approximates a function using second order Taylor expansion

$$J(w_t + p) \approx J(w_t) + p^T \nabla J(w_t) + \frac{1}{2} p^T \nabla^2 J(w_t) p$$



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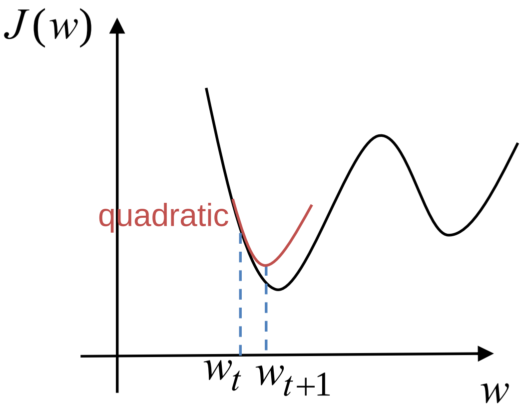

minimizing w.r.t. p

Hessian

$$p = \left(\nabla^2 J(w_t)\right)^{-1} \nabla J(w_t) = H_t^{-1} \nabla J(w_t)$$

$$w_{t+1} = w_t - H_t^{-1} \nabla J(w_t)$$

- No explicit step-length parameter
- If Hessian is not positive definite, Newton step may be undefined or may even diverge
- For quadratic functions, converges in a single step !

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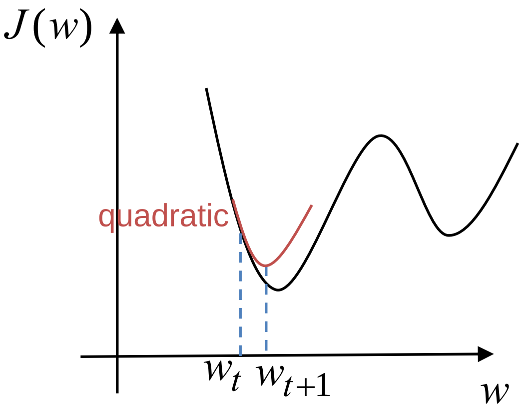

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Rate of Convergence: Quadratic

$$\frac{\|w_{t+1} - \hat{w}\|}{\|w_t - \hat{w}\|^2} \leq k$$

Fast convergence but each iteration slow: $O(d^2)$ space and $O(d^3)$ time

Quasi-Newton Methods

Do not require computation of Hessian but still super-linear convergence

Key Idea: Approximate Hessian locally using change in gradients

Secant equation

Approx Hessian → $B_{t+1} s_t = y_t$

$$s_t = w_{t+1} - w_t, \quad y_t = \nabla J(w_{t+1}) - \nabla J(w_t)$$

Wolfe's conditions

$$s_t^T y_t > 0$$

$$B_t \succ 0$$

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- Additional conditions imposed on B, e.g., symmetry or diagonal
- Difference between successive B's is low-rank
- BFGS (Broyden-Fletcher-Goldfarb-Shanno): uses rank-2 (inverse) Hessian updates

if $\tilde{B}_t = B_t^{-1}$ $\quad \tilde{B}_{t+1} = \arg\min_{\tilde{B}} \left\| \tilde{B} - \tilde{B}_t \right\|_F$ subject to $\tilde{B}_{t+1} = \tilde{B}_{t+1}^T, \quad \tilde{B}_{t+1} y_t = s_t$

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- Inverse of approx Hessian updated directly → $O(d^2)$ space and time

$$\tilde{B}_{t+1} = (I - \rho_t s_t y_t^T)\tilde{B}_t (I - \rho_t y_t s_t^T) + \rho_t s_t s_t^T \qquad \rho_t = 1/s_t^T y_t, \; \tilde{B}_0 = I$$

$O(d^2)$ cost per iteration, superlinear rate of convergence, self-correcting properties

Limited-Memory BFGS (L-BFGS)

Quasi-Newton methods produce dense Hessian approximations even when true Hessian is sparse → high storage cost for large-scale problems

Key Idea: Store approx Hessian using a few d-dim vectors from most recent iterations → Store at most m most recent pairs (s_t, y_t)

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$$w_{t+1} = w_t - \alpha_t \tilde{B}_t \nabla J(w_t)$$

- Iteratively estimate the product $\tilde{B}_t \nabla J(w_t)$ using most recent (s_t, y_t)
- Can be achieved efficiently in two loops in $O(md)$
- Different initialization for each inner loop possible, e.g.,

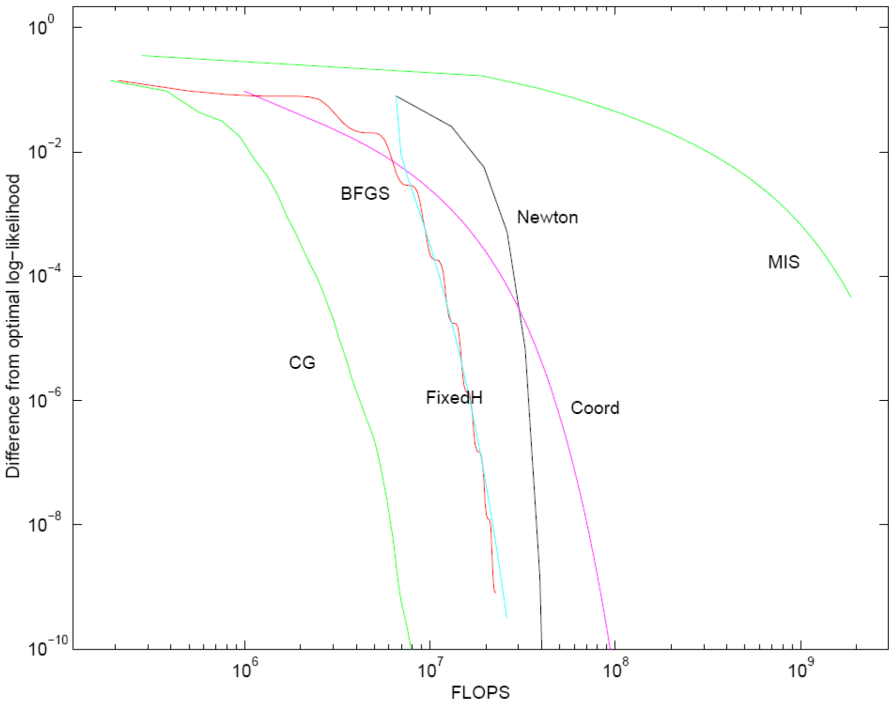
$$\tilde{B}_t^0 = \gamma_t I, \qquad \gamma_t = \frac{s_{t-1}^T y_{t-1}}{y_{t-1}^T y_{t-1}}$$

Similar to Conjugate-Gradient, rate of convergence linear instead of superlinear as in BFGS

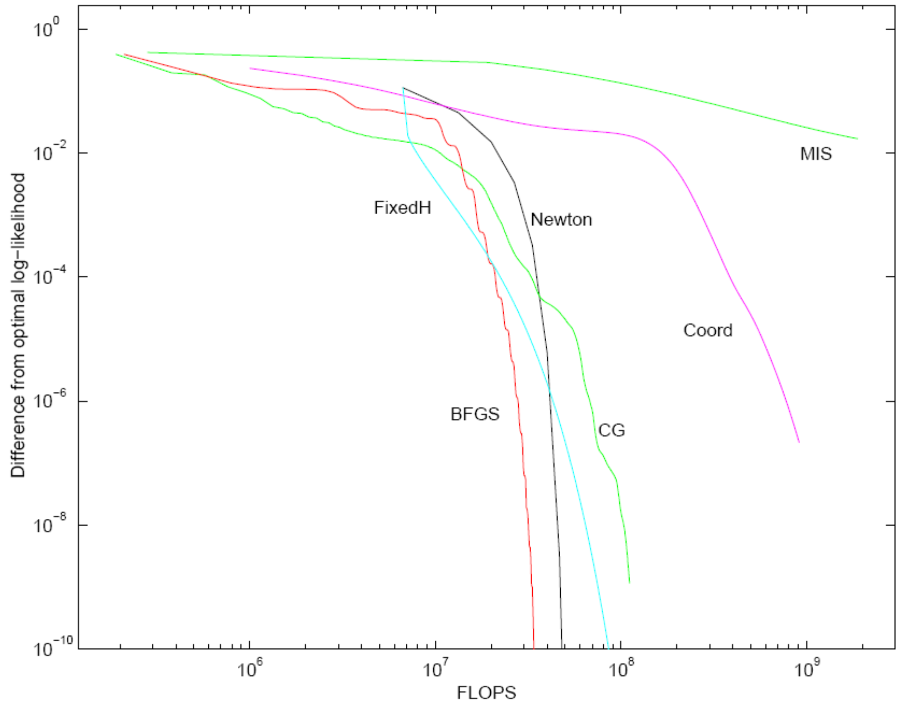
How about sparse, sampling-based or diagonal approximation of Hessian ?

Comparison: Logistic Regression

n=1500, d=100



independent features



correlated features

Hessian-based methods do better

Trade-off between number of iterations and cost per iteration !

Minka [5]

Batch vs Online

Most optimization functions use i.i.d. training data as,

Linear Regression $J(w) = \sum_i [(w^T x_i - y_i)^2 + \lambda w^T w]$

SVM $J(w) = \sum_i [\max(0, 1 - y_i w^T x_i) + \lambda w^T w]$

Logistic Regression $J(w) = -\sum_i [\log(\sigma(y_i w^T x_i) + \lambda w^T w]$

Batch methods

- compute gradients using all the training data
- each iteration needs to use full batch of data → slow for large datasets

Online (Stochastic) Methods

- use gradients from a small subset of data, usually just a single point
- do not decrease the function value monotonically
- typically have worse convergence properties than batch methods
- quite appropriate for large-scale applications where data is usually redundant
- can converge even before seeing all the data once → very fast
- popular conjecture: may also avoid bad local minima

Stochastic Gradient Descent (SGD)

At each iteration, use a small training subset to estimate the gradient

$$w_{t+1} = w_t - \eta_t \nabla J(w_t, x_t)$$

single point or a small subset of training data

Stochastic Gradient Descent (SGD)

At each iteration, use a small training subset to estimate the gradient

$$w_{t+1} = w_t - \eta_t \nabla J(w_t, x_t)$$

single point or a small subset of training data

Converges to optimal value $\hat{w}$ if,

parameters may move arbitrary distances $\sum_t \eta_t = \infty$

step size decreases fast enough $\sum_t \eta_t^2 < \infty$

Step-length $\eta_t = \frac{\tau}{\tau + t}\eta_0$ $\tau, \eta_0 > 0$ are tuning parameters

Properties

- $O(d)$ space and time per iteration instead of $O(nd)$ of gradient descent
- Outperforms batch gradient methods on large datasets
- Slow convergence on ill-conditioned problems
- Stochastic Meta-Descent: adjust a different gain for each parameter

Experiment - SGD

SVM classification task

d = 47K (~80 nonzero), n = ~800K

Model	Algorithm	Training Time	Objective	Test Error
Hinge loss, $\lambda = 10^{-4}$ *See [21,22].*	SVMLight	23,642 secs	0.2275	6.02%
	SVMPerf	66 secs	0.2278	6.03%
	SGD	**1.4 secs**	0.2275	6.02%
Logistic loss, $\lambda = 10^{-5}$ *See [23].*	LibLinear ($\rho = 10^{-2}$)	30 secs	0.18907	5.68%
	LibLinear ($\rho = 10^{-3}$)	44 secs	0.18890	5.70%
	SGD	**2.3 secs**	0.18893	5.66%

Bottou & Bousquet [8]

SGD for Sparse Data

Suppose training set vectors $\{x_i \in \Re^d\}_{i=1,\ldots,n}$ are sparse

- Only a small fraction (s) of d elements are non-zero $s << 1$
- Common for many applications: text, images, biological data,…

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Objective function $J(w) = \sum_{i=1}^{n} [L(y_i w^T x_i) + \lambda R(w)]$

$$\nabla J(w_t, x_t) = \underbrace{\nabla L(y_t w_t^T x_t) y_t x_t}_{\text{sparse}} + \underbrace{\lambda \nabla R(w_t)}_{\text{dense}}$$

} dense vector update $O(d)$ per iteration

How to make sparse updates, i.e., $O(sd)$ per iteration?

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How to make sparse updates, i.e., $O(sd)$ per iteration?

Break updates into two parts

1. Update using gradients of $L(.)$ alone ignoring the regularizer

$$w_{t+1} = w_t - \eta_t \nabla L(w_t, x_t)$$

2. Every kth iteration, adjust w using gradients of regularizer

$$w_{t+1} \leftarrow w_{t+1} - k\eta_t \nabla R(w_{t+1})$$

Perceptron

Originally proposed to learn a linear binary classifier $y = \{-1, 1\}$

$$f(x) = \mathrm{sgn}(w^T x)$$

Update Rule

$$w_{t+1} = \begin{cases} w_t + y\,x_t & \text{if } x \text{ is misclassified, i.e., } y \neq f(x) \\ w_t & \text{otherwise} \end{cases}$$

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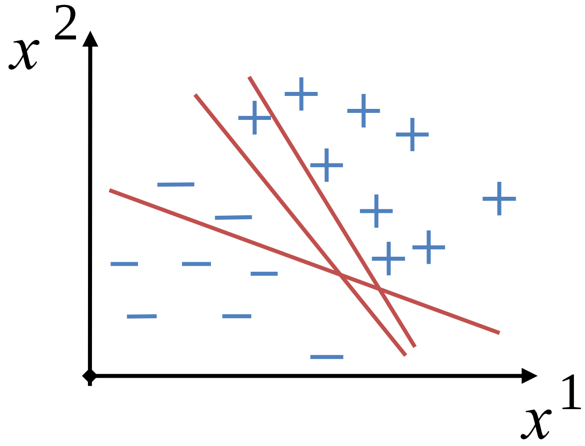

Properties

- Stochastic gradient descent on a non-differentiable loss function
- Guaranteed to converge if data is linearly separable
- What happens for inseparable data ?

will not converge but oscillate !

- Use of heuristics such as voting with various parameter vectors

Natural Gradient Descent

Incorporate Riemannian Metric into stochastic descent

$$G_t = E_x[\nabla J(w_t, x_t) \nabla J(w_t, x_t)^T]$$

$$w_{t+1} = w_t - \eta_t \tilde{G}_t^{-1} \nabla J(w_t, x_t)$$

$$\eta_t = \frac{\tau}{\tau + t} \eta_0$$

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Metric update $$\tilde{G}_{t+1} = (t-1)/t\ \tilde{G}_t + (1/t)\nabla J(w_t, x_t)\nabla J(w_t, x_t)^T$$

assuming Hessian to be constant

Properties

- Update matrix inverse directly → $O(d^2)$ space and time per iteration
- More stable – has good theoretical properties
- Still expensive for large-scale problems

Online-BFGS

Change of gradients estimated using a subset of training data

$\tilde{B}_{t+1} y_t = s_t$

$s_t = w_{t+1} - w_t,$

$y_t = \nabla J(w_{t+1}) - \nabla J(w_t)$

$$w_{t+1} = w_t - \eta_t \tilde{B}_t \nabla J(w_t, x_t)$$

stochastic approximation of inverse Hessian

Wolfe's conditions

$s_t^T y_t > 0$

$B_t \succ 0$

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1. To maintain positive curvature

Modify $y_t = \nabla J(w_{t+1}, x_t) - \nabla J(w_t, x_t) + \lambda s_t \quad \lambda \geq 0$ Compute on the same sample !

2. Initialize $\tilde{B}$ using a small coefficient to restrict initial parameter update

$$\tilde{B}_0 = \varepsilon I \qquad \varepsilon \approx 10^{-10}$$

3. Modify the update of $\tilde{B}_{t+1}$

$\rho_t = 1/s_t^T y_t$

$$\tilde{B}_{t+1} = (I - \rho_t s_t y_t^T) \tilde{B}_t (I - \rho_t s_t y_t^T) + c \rho_t s_t s_t^T \qquad 0 < c \leq 1 \quad \eta_t = \eta_t / c$$

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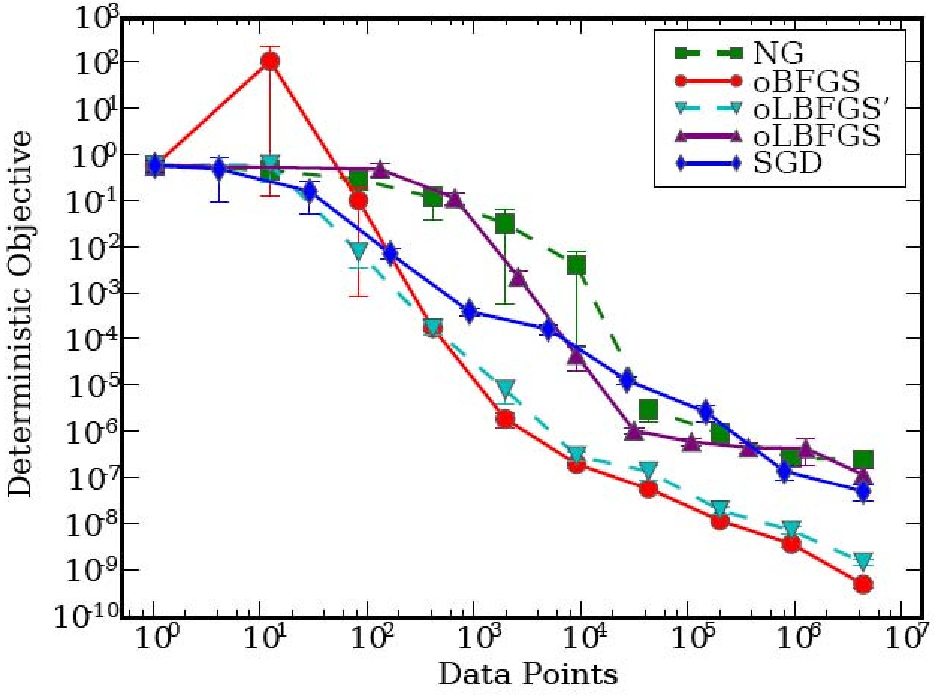
- Test of convergence: If last k stochastic gradients have been below a threshold
- Online version of L-BFGS possible → $O(md)$ cost instead of $O(d^2)$

Experiments

Synthetic quadratic function

parameters d = 5, n = ~1M

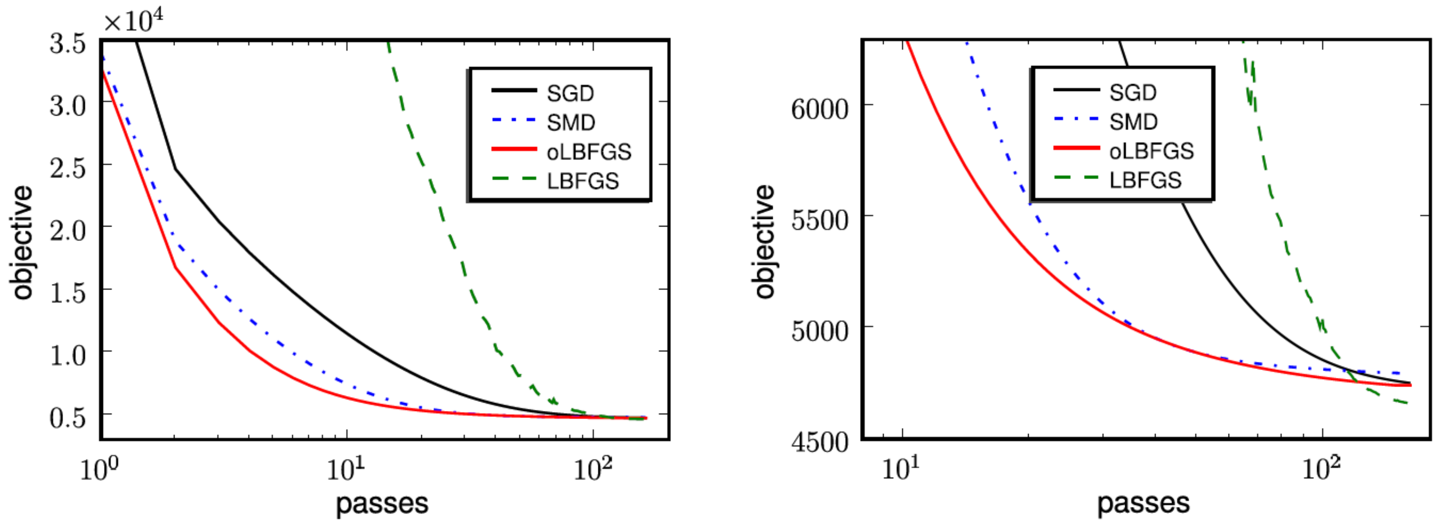


Schraudolph et al. [7]

Experiments

On Conditional Random Field (CRF) applied to text chunking

parameters d = 100K, n = ~9K



Schraudolph et al. [7]

Stochastic Gradient Descent (Quasi-Newton)

Approximate inverse Hessian by a diagonal matrix

Inspired by online-BFGS

$\tilde{B}_{t+1} y_t = s_t$

$s_t = w_{t+1} - w_t,$

$y_t = \nabla J(w_{t+1}) - \nabla J(w_t)$

$$w_{t+1} - w_t \approx \tilde{B}_{t+1}(\nabla J(w_{t+1}, x_t) - \nabla J(w_t, x_t))$$

diagonal matrix

Wolfe's conditions

$s_t^T y_t > 0$

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diagonal matrix

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$$s_t^T y_t > 0$$
$$B_t \succ 0$$

$$[w_{t+1} - w_t]_i \approx \tilde{B}_{ii}[\nabla J(w_{t+1}, x_t) - \nabla J(w_t, x_t)]_i$$

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In Practice,

- Update matrix entries only every k iterations
- Do a leaky average of B to get stable updates

$$\tilde{B}_{ii} \leftarrow \tilde{B}_{ii}[1 + k\tilde{B}_{ii} r_i]^{-1}$$

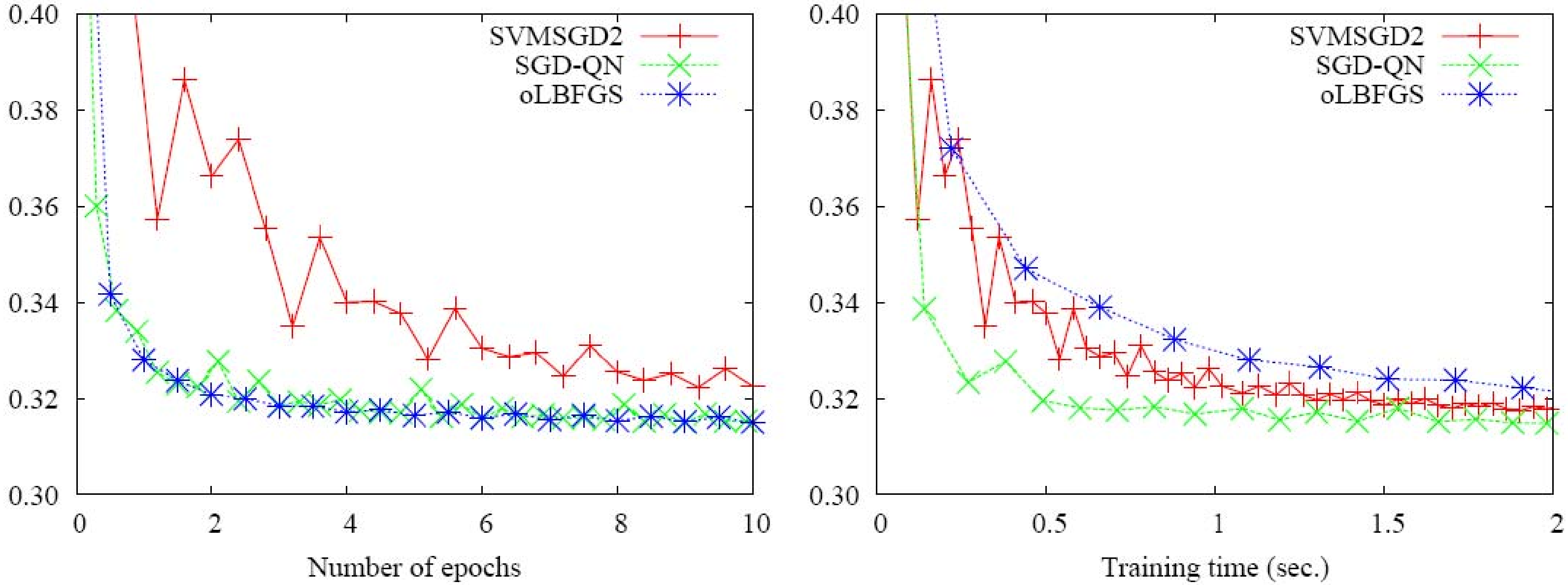
$r_i = [\nabla J(w_{t+1}, x_t) - \nabla J(w_{t-k}, x_t)]_i / [w_{t+1} - w_t]_i \quad r_i \leftarrow \max\{\lambda, \min\{100\lambda, r_i\}\}$

- Has a flavor of partially 'fixed-Hessian'

Stochastic Gradient Descent (Quasi-Newton)

Alpha dataset of Pascal Challenge (2008)

parameters d = 500 (dense), n = ~100K



	ALPHA	RCV1
SGD	0.13	36.8
SVMSGD2	0.10	0.20
SGD-QN	0.21	0.37

sparse SGD → SVMSGD2

RCV1: d = 47K, s = 0.0016

Bordes et al. [9]

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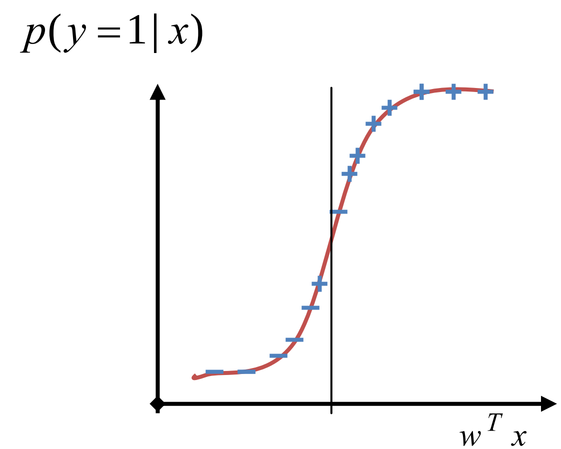
Logistic Regression

Given: A labeled training set, $\{x_i, y_i\}_{i=1 \ldots n} \quad x_i \in \Re^d, y_i \in \{-1, 1\}$

Goal: Learn a predictive function $p(y=1 | x) = \sigma(w^T x)$ Absorb w_0 in w

$$p(y_i | x_i) = \sigma(y_i w^T x_i)$$



(negative) log-posterior

$$L(w) = \underbrace{\sum_i \log(1 + \exp(-y_i w^T x_i))}_{\text{log-likelihood}} + \underbrace{\lambda w^T w}_{\text{log-prior}}$$

Convex problem, Newton method:

$$w_{t+1} = (XAX^T + \lambda I)^{-1} XAz$$

$n \sim O(100M), d \sim O(100K)$

$O(nd^2)$ multiplication

$O(d^3)$ inversion

$O(nd)$ First-order methods