Gradient Decent and such

Schwartz

April 13, 2017

A brief history of Optimization

- 300 bc Euclid considers minimal distance from point to a line & proves square is the greatest area rectangle
- 1615 Kepler optimizes dimensions of wine barrel & formulates an early version of the (classical) secretary problem while looking for a new wife
- 1636 Fermat shows derivatives vanish at extremes & light travels between two points in minimal time
- 1660s Newton & Leibniz create the mathematical basis of calculus and hence optimization calculus
- 1696 Johann & Jacob Bernoulli study Brachistochrone problem – calculus optimization is born
- 1712 König shows that the shape of honeycomb is optimal. The French Academy of Sciences declares the phenomenon as divine guidance
- 1740 Euler's publication begins the research on a general theory of calculus optimization
- 1754 Lagrange makes his first of many findings regarding calculus optimization at age 19
- 1900's The first optimization algorithms are presented by Weierstrass, Steiner, Hamilton and Jacobi
- 1806 Legendre presents the least square method, which also Gauss claims to have invented
- 1815 "The Law of Diminishing Returns" (introduced simultaneously by Malthus, Torrens, West, and Ricardo) uses a (quasi) concave function
- 1826 Fourier formulates linear programming (LP) for solving mechanics and probability problems
- 1847 Cauchy presents the gradient method
- 1857 Gibbs shows chemical equilibrium is minimum energy
- 1870s The marginalist revolution in economics shifts the focus of economists to maximizing individuals utility
- 1880s Convexity theory created – Jensen introduces convex functions in 1905 – Minkowski convex sets in 1911
- 1917 Hancock publishes the first text book on optimization: "Theory of Minima and Maxima"
- 1917 Thompson's "On Growth and Form" applies optimization to analyze the forms of living organisms
- 1928 Ramsey studies optimal economic growth which becomes optimal growth theory in the 1950's
- 1932 Menger generalizes the traveling salesman problem
- 1939 Kantorovich presents LP-model & solution algorithm and receives Nobel prize in 1975 with Koopmans
- 1944 Neuman and Morgenstern, and Wald (1947) solve sequential problems w/ dynamic programming (DP)
- 1947 Dantzig (USAF) presents the Simplex method for LP-problems, Neumann establishes duality theory
- 1950's Electronic calculation initiates algorithmic research
- 1951 Markowitz presents portfolio theory using quadratic programing (QP) and receives the 1990 Nobel prize
- 1954 Ford & Fulkerson introduce combinatorial optimization for network research problems
- 1960's Space race sparks optimal control theory research
- 1970s Complexity analysis influences optimization theory
- 1980's Heuristic global optimization algorithms for large scale problems gain popularity as computers improve

Objectives

- Loss Function
- Cost Function
- Objective Function

- Gradient Decent
- Stochastic Gradient Descent
- Newton's Method

Exercise of the day

Find parameters that maximizes the fit of model to data

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minimize distance between
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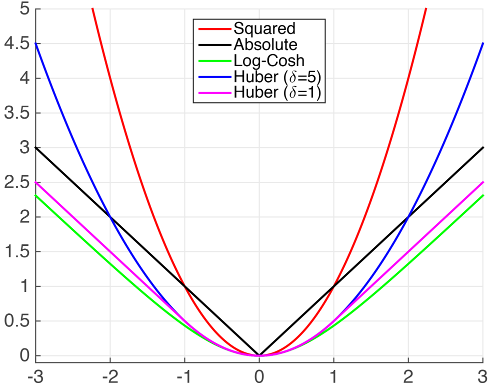
$$\hat{Y}_i \approx Y_i$$

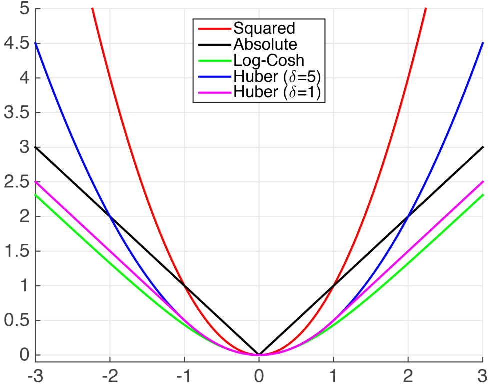
Regression Loss Functions

$$Y_i - \hat{Y}_i$$



Regression Loss Functions

$$(Y_i - \hat{Y}_i)^2$$



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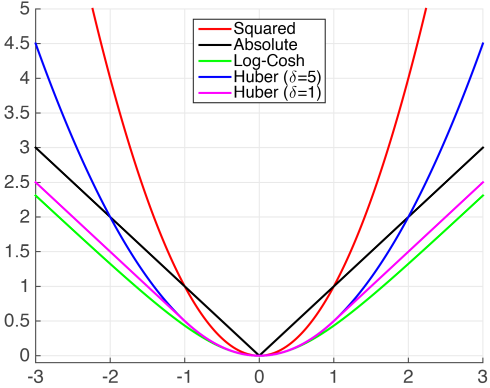

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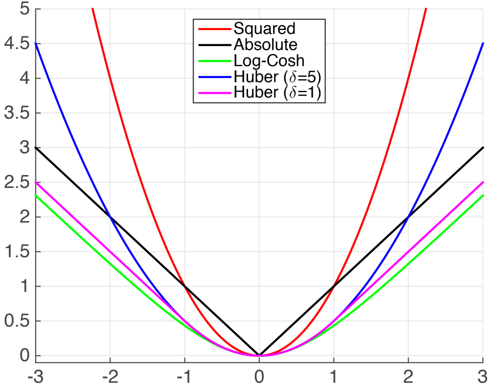
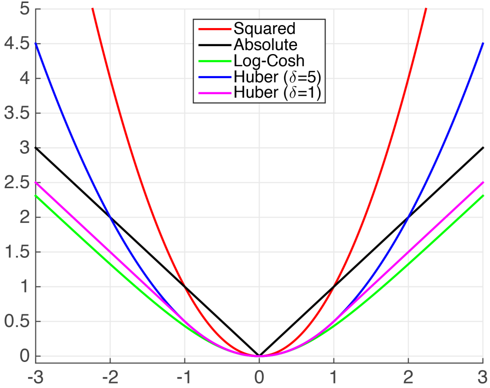
$$ln(cosh(Y_i - \hat{Y}_i))$$



Regression Loss Functions

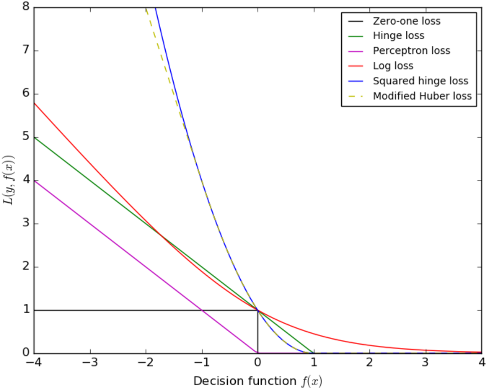
$$L_\delta(Y_i - \hat{Y}_i)$$

$$L_\delta(a) = \begin{cases} \frac{1}{2}a^2 & : |a| < \delta \\ \delta(|a| - \frac{1}{2}\delta) & : o.w. \end{cases}$$



Classification Loss Functions

$$Y \in [0,1] : \min_p - Y \log p - (1 - Y) \log(1 - p) \qquad p = \frac{1}{1 + e^{-x^T \beta}}$$



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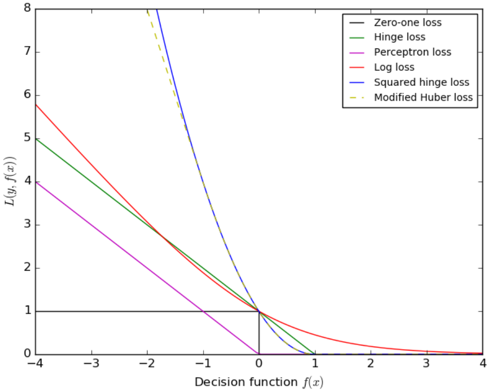
$$Y \in [-1,1] : \min_p \frac{1}{ln2}\left(1 + e^{-Yln\left(\frac{p}{1-p}\right)}\right) \qquad ln\left(\frac{p}{1-p}\right) = x^T\beta$$



Cost function

- $\sum(Y_i - x_i^T\beta)^2$

- $-\sum Y_i \log g^{-1}(x_i^T\beta) + (1 - Y_i)\log\left(1 - g^{-1}(x_i^T\beta)\right)$

$$g^{-1}(z) = \frac{1}{1 + e^{-z}}$$

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  Regularized cost functions also don't have closed form solutions

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or

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- But in Machine Learning
  the standard orientation and nomenclature is "minimize cost"

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For some function $f(\boldsymbol{x})$, the gradient

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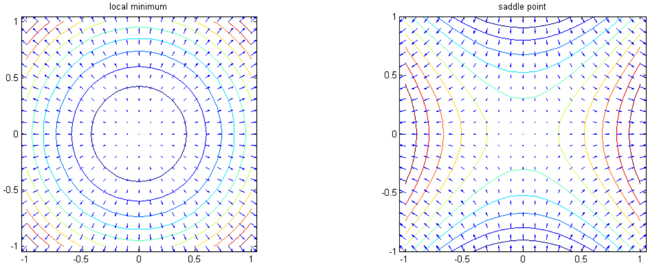

Gradient Descent

http://vis.supstat.com/2013/03/gradient-descent-algorithm-with-r/

0. Choose step size α and precision threshold ϵ
1. Select starting point $\boldsymbol{x}^{(0)}$, set $i = 1$
2. Update $\boldsymbol{x}^{(t)} = \boldsymbol{x}^{(t-1)} - \alpha \nabla f(\boldsymbol{x}^{(t-1)})$
3. If $\frac{|f(\boldsymbol{x}^{(t-1)})| - |f(\boldsymbol{x}^{(t)})|}{|f(\boldsymbol{x}^{(t-1)})|} < \epsilon$, return *min* $|f(\boldsymbol{x}^{(t)})|$ & *argmin* $\boldsymbol{x}^{(t)}$
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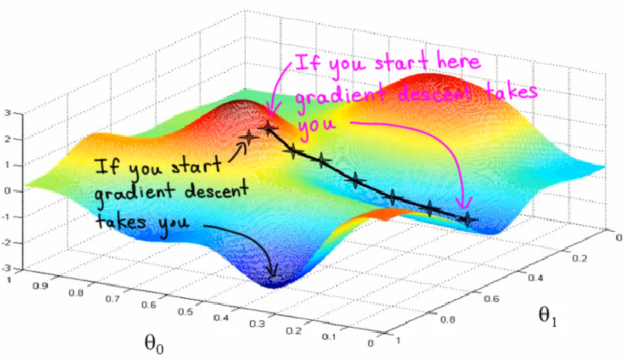
c. $|\nabla f| < \epsilon$

Pitfalls (literally)



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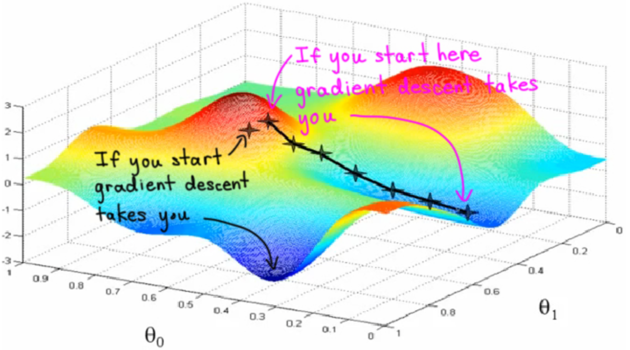

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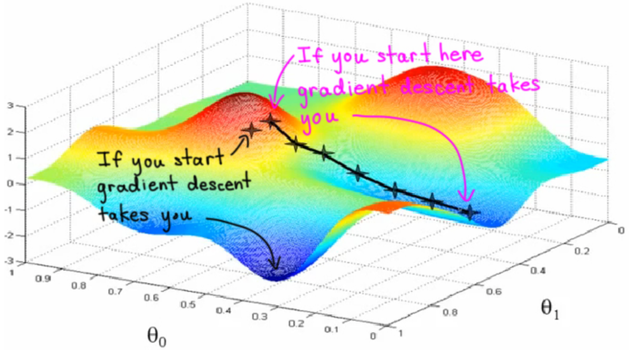

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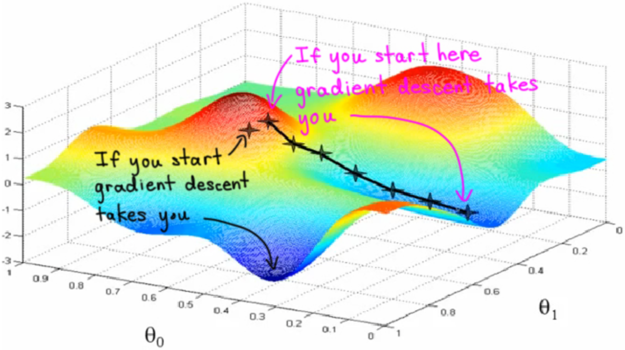

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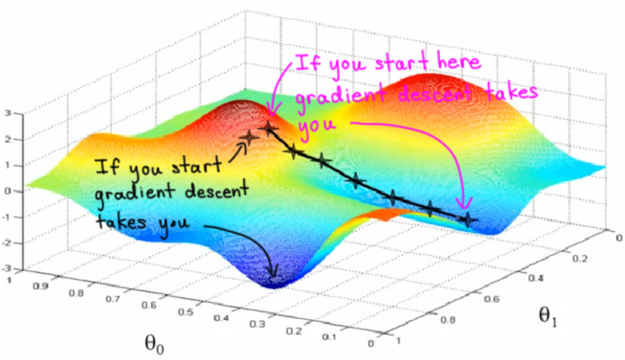

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- good performance requires feature scaling & parameter tuning

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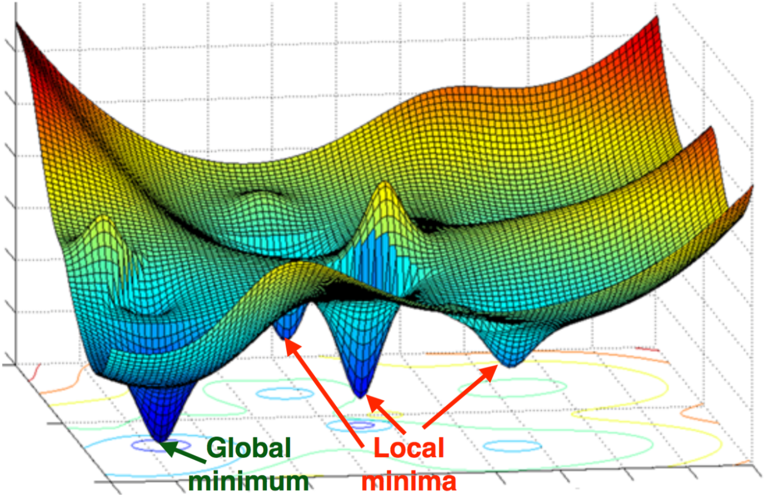

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$$\nabla L(\beta) = ?$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

$$\nabla L(\beta) = ?$$

$$\frac{d}{dz} g^{-1}(z) = \frac{d}{dz} \frac{1}{1 + e^{-z}}$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

$$\nabla L(\beta) = ?$$

$$\begin{aligned} \frac{d}{dz} g^{-1}(z) &= \frac{d}{dz} \frac{1}{1 + e^{-z}} \\ &= \frac{d}{dz} (1 + e^{-z})^{-1} \end{aligned}$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

$$\nabla L(\beta) = ?$$

$$\begin{aligned}
\frac{d}{dz} g^{-1}(z) &= \frac{d}{dz} \frac{1}{1 + e^{-z}} \\
&= \frac{d}{dz} (1 + e^{-z})^{-1} \\
&= -(1 + e^{-z})^{-2} (-e^{-z})
\end{aligned}$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

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&= \frac{d}{dz} (1 + e^{-z})^{-1} \\
&= -(1 + e^{-z})^{-2} (-e^{-z}) \\
&= \frac{1}{1 + e^{-z}} \frac{e^{-z}}{1 + e^{-z}}
\end{aligned}$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

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&= \frac{d}{dz} (1 + e^{-z})^{-1} \\
&= -(1 + e^{-z})^{-2} (-e^{-z}) \\
&= \frac{1}{1 + e^{-z}} \frac{e^{-z}}{1 + e^{-z}} \\
&= g^{-1}(z) \left(1 - g^{-1}(z)\right)
\end{aligned}$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

$$\nabla L(\beta) = ?$$

$$\frac{\partial}{\partial \beta_{\color{red}{j}}} L(\beta)$$

$$= \frac{\partial}{\partial \beta_j} \left(\sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)\right)$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

$$\nabla L(\beta) = ?$$

$$\begin{aligned}
&\frac{\partial}{\partial \beta_{j}} L(\beta) \\
&= \frac{\partial}{\partial \beta_j} \left(\sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)\right) \\
&= \sum \frac{\partial}{\partial \beta_j} g^{-1}(x_i^T \beta) \left(\frac{Y_i}{g^{-1}(x_i^T \beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T \beta))}\right)
\end{aligned}$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

$$\nabla L(\beta) = ?$$

$$\begin{aligned}
&\frac{\partial}{\partial \beta_j} L(\beta) \\
&= \frac{\partial}{\partial \beta_j} \left(\sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)\right) \\
&= \sum \frac{\partial}{\partial \beta_j} g^{-1}(x_i^T \beta) \left(\frac{Y_i}{g^{-1}(x_i^T \beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T \beta))} \right) \\
&= \sum g^{-1}(x_i^T \beta) \left(1 - g^{-1}(x_i^T \beta)\right) x_{ij} \left(\frac{Y_i}{g^{-1}(x_i^T \beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T \beta))} \right)
\end{aligned}$$

Logistic regression

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&= \sum \frac{\partial}{\partial \beta_j} g^{-1}(x_i^T \beta) \left(\frac{Y_i}{g^{-1}(x_i^T \beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T \beta))}\right) \\
&= \sum g^{-1}(x_i^T \beta) \left(1 - g^{-1}(x_i^T \beta)\right) x_{ij} \left(\frac{Y_i}{g^{-1}(x_i^T \beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T \beta))}\right) \\
&= \sum x_{ij} \left(Y_i \left(1 - g^{-1}(x_i^T \beta)\right) - (1 - Y_i) g^{-1}(x_i^T \beta)\right)
\end{aligned}$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T\beta) + (1 - Y_i)\log\left(1 - g^{-1}(x_i^T\beta)\right)$$

$$\nabla L(\beta) = ?$$

$$\begin{aligned}
&\frac{\partial}{\partial \beta_j} L(\beta) \\
&= \frac{\partial}{\partial \beta_j}\left(\sum Y_i \log g^{-1}(x_i^T\beta) + (1 - Y_i)\log\left(1 - g^{-1}(x_i^T\beta)\right)\right) \\
&= \sum \frac{\partial}{\partial \beta_j} g^{-1}(x_i^T\beta)\left(\frac{Y_i}{g^{-1}(x_i^T\beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T\beta))}\right) \\
&= \sum g^{-1}(x_i^T\beta)\left(1 - g^{-1}(x_i^T\beta)\right) x_{ij}\left(\frac{Y_i}{g^{-1}(x_i^T\beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T\beta))}\right) \\
&= \sum x_{ij}\left(Y_i\left(1 - g^{-1}(x_i^T\beta)\right) - (1 - Y_i)g^{-1}(x_i^T\beta)\right) \\
&= \sum x_{ij}\left(Y_i - g^{-1}(x_i^T\beta)\right) = \sum_{i=1}^{n} x_{ij}\left(Y_i - \frac{1}{1 + e^{-x_i^T\beta}}\right) = \sum_{i=1}^{n} x_{ij}(Y_i - \hat{Y}_i)
\end{aligned}$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T\beta) + (1 - Y_i)\log\left(1 - g^{-1}(x_i^T\beta)\right) \; - \lambda\frac{1}{2}||\beta||^2$$

$$\nabla L(\beta) = ?$$

$$\frac{\partial}{\partial \beta_j} L(\beta)$$

$$= \frac{\partial}{\partial \beta_j}\left(\sum Y_i \log g^{-1}(x_i^T\beta) + (1 - Y_i)\log\left(1 - g^{-1}(x_i^T\beta)\right)\right)$$

$$= \sum \frac{\partial}{\partial \beta_j} g^{-1}(x_i^T\beta)\left(\frac{Y_i}{g^{-1}(x_i^T\beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T\beta))}\right)$$

$$= \sum g^{-1}(x_i^T\beta)\left(1 - g^{-1}(x_i^T\beta)\right) x_{ij} \left(\frac{Y_i}{g^{-1}(x_i^T\beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T\beta))}\right)$$

$$= \sum x_{ij}\left(Y_i\left(1 - g^{-1}(x_i^T\beta)\right) - (1 - Y_i)g^{-1}(x_i^T\beta)\right)$$

$$= \sum x_{ij}\left(Y_i - g^{-1}(x_i^T\beta)\right) = \sum_{i=1}^{n} x_{ij}\left(Y_i - \frac{1}{1 + e^{-x_i^T\beta}}\right) = \sum_{i=1}^{n} x_{ij}(Y_i - \hat{Y}_i)$$

Logistic regression

$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T\beta) + (1 - Y_i)\log\left(1 - g^{-1}(x_i^T\beta)\right) - \lambda|\beta|$$

$$\nabla L(\beta) = ?$$

$$\begin{aligned}
&\frac{\partial}{\partial \beta_j} L(\beta)\\
&= \frac{\partial}{\partial \beta_j}\left(\sum Y_i \log g^{-1}(x_i^T\beta) + (1 - Y_i)\log\left(1 - g^{-1}(x_i^T\beta)\right)\right)\\
&= \sum \frac{\partial}{\partial \beta_j} g^{-1}(x_i^T\beta)\left(\frac{Y_i}{g^{-1}(x_i^T\beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T\beta))}\right)\\
&= \sum g^{-1}(x_i^T\beta)\left(1 - g^{-1}(x_i^T\beta)\right) x_{ij}\left(\frac{Y_i}{g^{-1}(x_i^T\beta)} - \frac{(1 - Y_i)}{(1 - g^{-1}(x_i^T\beta))}\right)\\
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$$L(\beta) = \sum Y_i \log g^{-1}(x_i^T \beta) + (1 - Y_i) \log \left(1 - g^{-1}(x_i^T \beta)\right)$$

$$\nabla L(\beta) = \begin{bmatrix} \sum x_{i1} \left(Y_i - \frac{1}{1+e^{-x_i^T \beta}} \right) \\ \sum x_{i2} \left(Y_i - \frac{1}{1+e^{-x_i^T \beta}} \right) \\ \vdots \\ \sum x_{ip} \left(Y_i - \frac{1}{1+e^{-x_i^T \beta}} \right) \end{bmatrix}$$

$$\beta^{(t)} = \beta^{(k-1)} + \alpha \nabla f(\beta^{(k-1)})$$

Potential Gradient Decent Drawbacks

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- Memory (data needs to fit)
- Processor (cost function over all rows is expensive)

Potential Gradient Decent Drawbacks *Solutions*

- Observations contribute equal weight to the gradient

$$\frac{\partial L_{1,\cdots n}}{\partial \beta_j}(\beta) = \sum_{i=1}^{n} x_{ij} \left(Y_i - \frac{1}{1 + e^{-x_i^T \beta}} \right)$$

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- We could just use only a single data point at each iteration?

$$\frac{\partial L_i}{\partial \beta_j}(\beta) = x_{ij} \left(Y_i - \frac{1}{1 + e^{-x_i^T \beta}} \right)$$

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$$\frac{\partial L_i}{\partial \beta_j}(\beta) = x_{ij} \left(Y_i - \frac{1}{1+e^{-x_i^T \beta}} \right)$$

- The expected direction of the gradient would stay the same

$$\frac{1}{n} \mathrm{E}\left[\frac{\partial L_{1,\cdots n}}{\partial \beta_j}(\beta) \right] = \mathrm{E}\left[\frac{\partial L_i}{\partial \beta_j}(\beta) \right]$$

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  This would address memory/processing limitations

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  It has been empirically proven to also often converge faster!

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- We could also use a batch of data points at each iteration

  This would address memory/processing limitations
  It has been empirically proven to also often converge faster!
  It does tend to oscillate around as it nears the minimum...

Newton-Raphson

- Gradient Decent

$$x^{(t)} = x^{(t-1)} - \alpha f'(x^{(t-1)})$$

$$\boldsymbol{x}^{(t)} = \boldsymbol{x}^{(t-1)} - \alpha \nabla f(\boldsymbol{x}^{(t-1)})$$

Newton-Raphson

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$$\boldsymbol{x}^{(t)} = \boldsymbol{x}^{(t-1)} - \alpha \nabla f(\boldsymbol{x}^{(t-1)})$$

- Newton-Raphson

$$x^{(t)} = x^{(t-1)} - \frac{f'(x^{(t-1)})}{f''(x^{(t-1)})}$$

$$\boldsymbol{x}^{(t)} = \boldsymbol{x}^{(t-1)} - [Hf(\boldsymbol{x}^{(t-1)})]^{-1} \nabla f(\boldsymbol{x}^{(t-1)})$$

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2nd order information makes Newton-Raphson faster

Newton-Raphson

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2nd order information makes Newton-Raphson faster
Inverting the Hessian matrix can be costly (or impossible)

Newton-Raphson

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2nd order information makes Newton-Raphson faster
Inverting the Hessian matrix can be costly (or impossible)
Newton-Raphson can diverge with an initial bad guess

Conclusions

- Best Method?

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  Depends

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- So why are we doing this?

Conclusions

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  Depends
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  Probably not
- So why are we doing this?

  Fitting models is just optimizing... knowing how it works could help you apply model fitting procedures more effectively

Bonus

http://cs229.stanford.edu/notes/cs229-notes1.pdf