Gradient Decent and such

Schwartz

December 21, 2016

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

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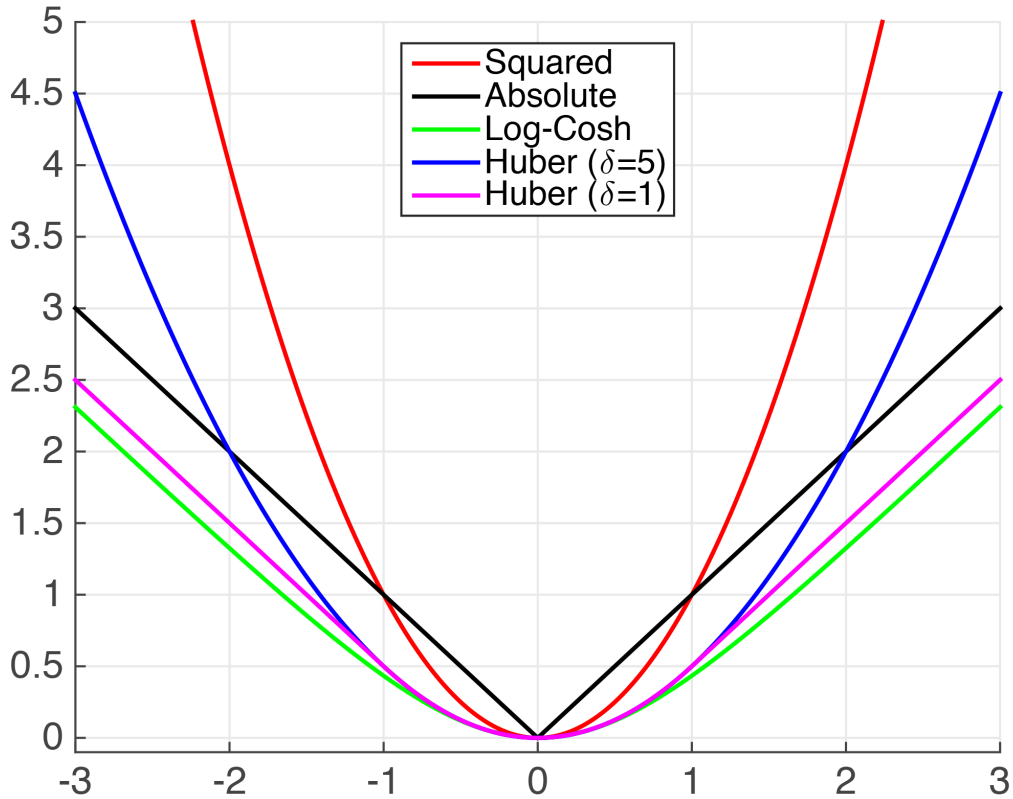
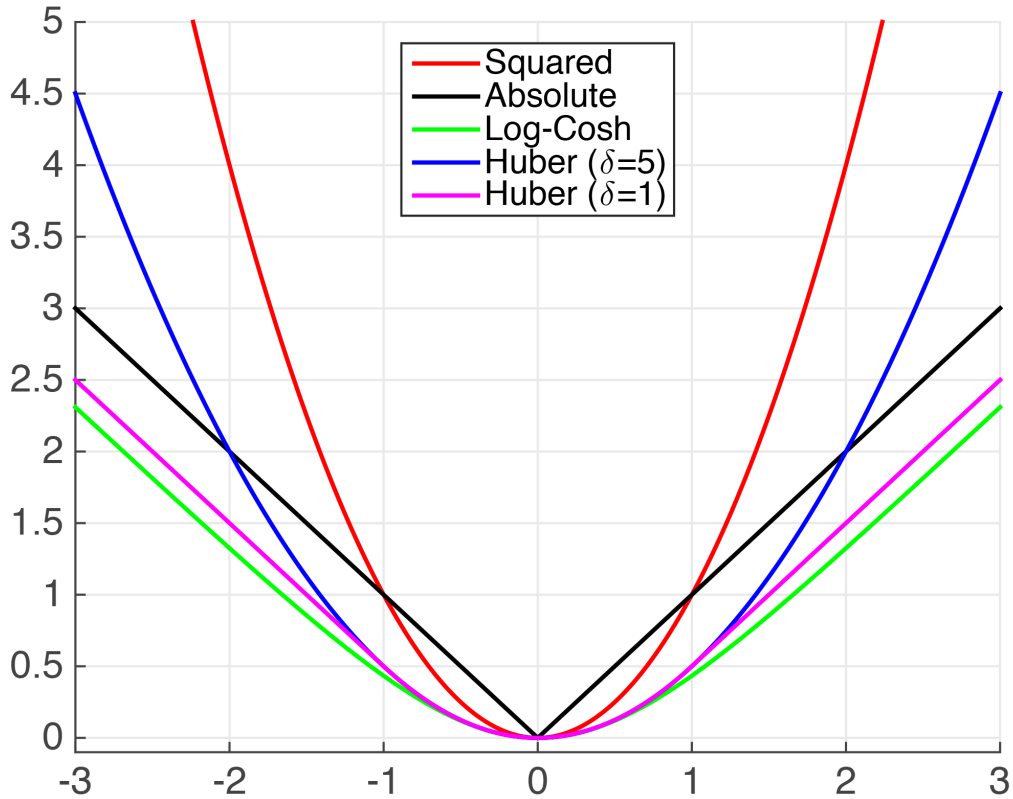
Regression Loss Functions

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



Regression Loss Functions

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



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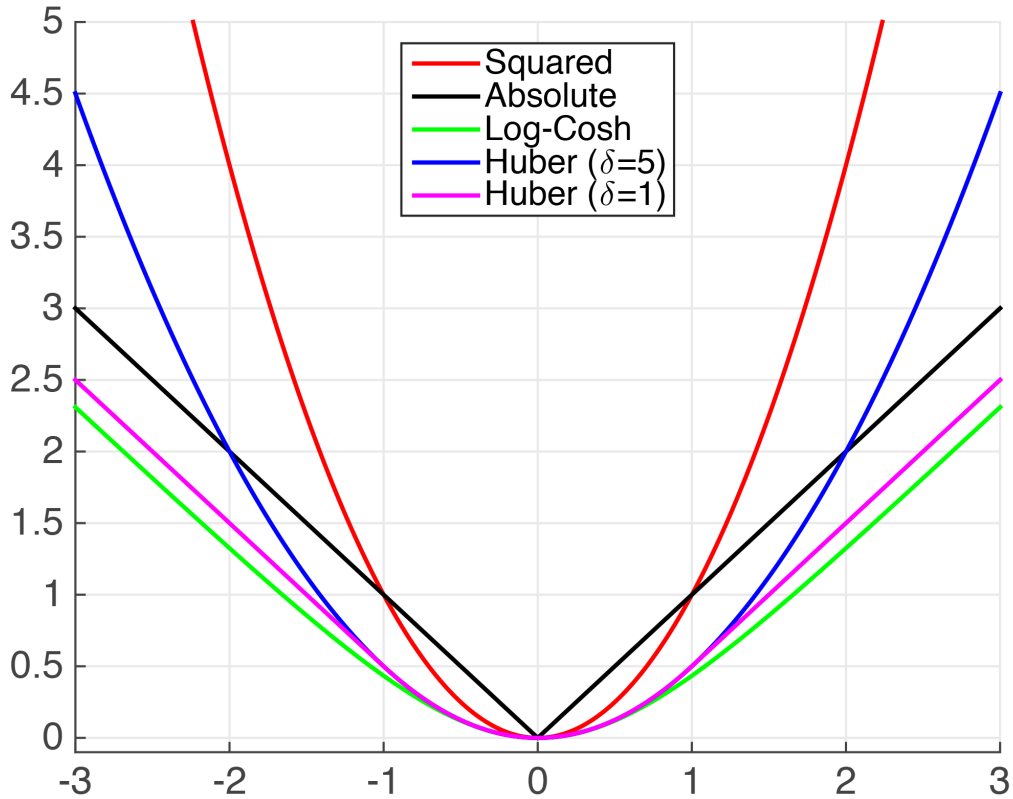
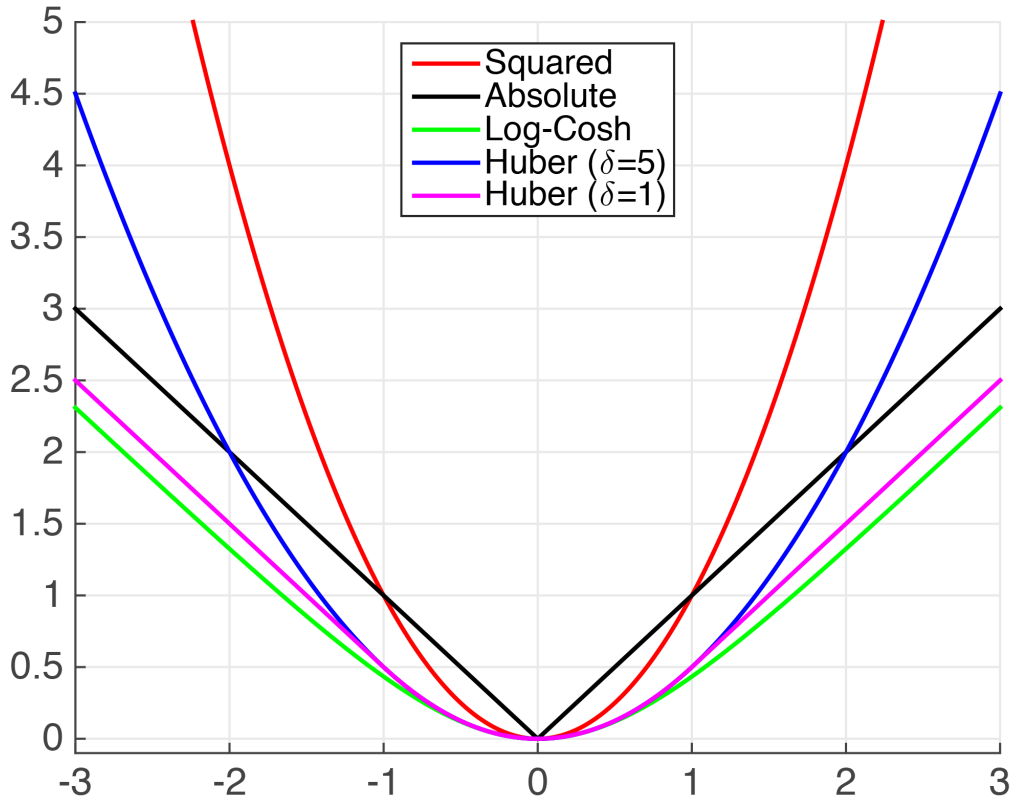
$$|Y_i - \hat{Y}_i|$$



Regression Loss Functions

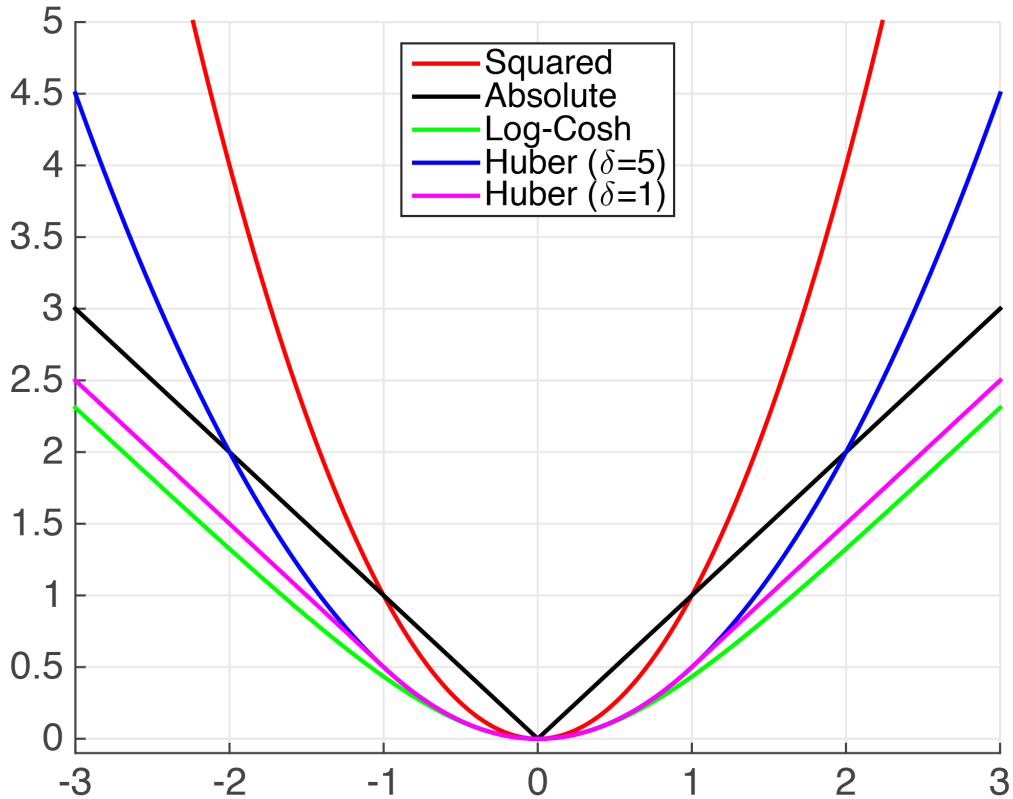
$$ln(cosh(Y_i - \hat{Y}_i))$$



Regression Loss Functions

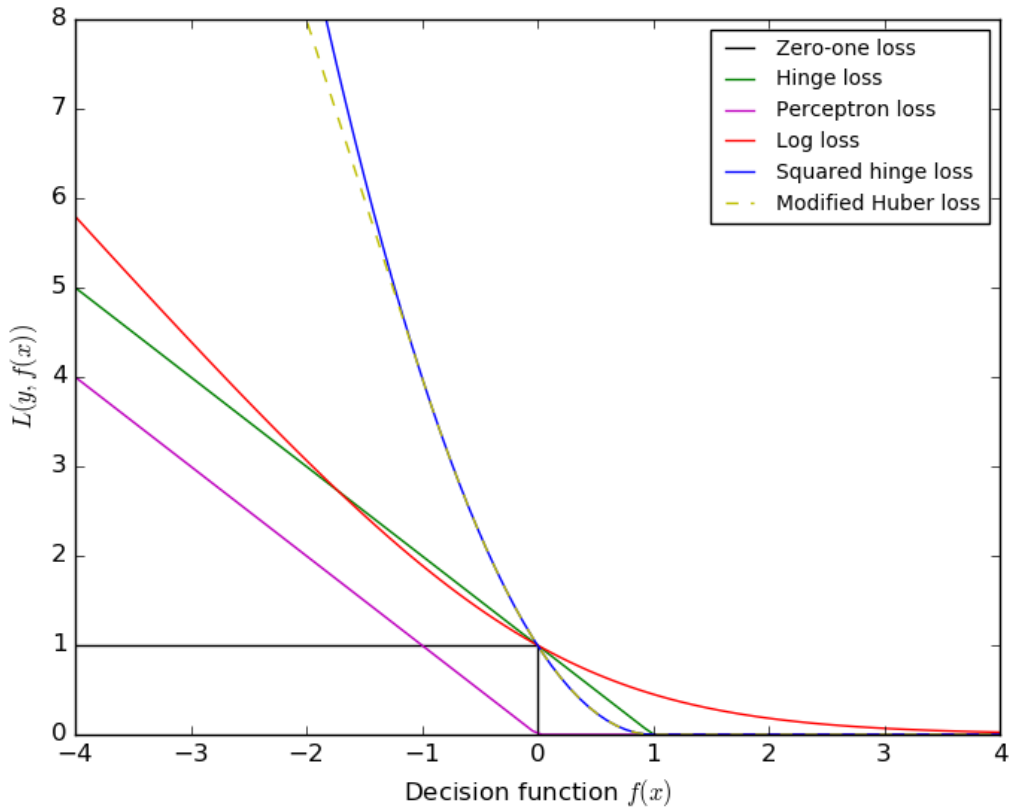
$$L_\delta(Y_i - \hat{Y}_i)$$

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



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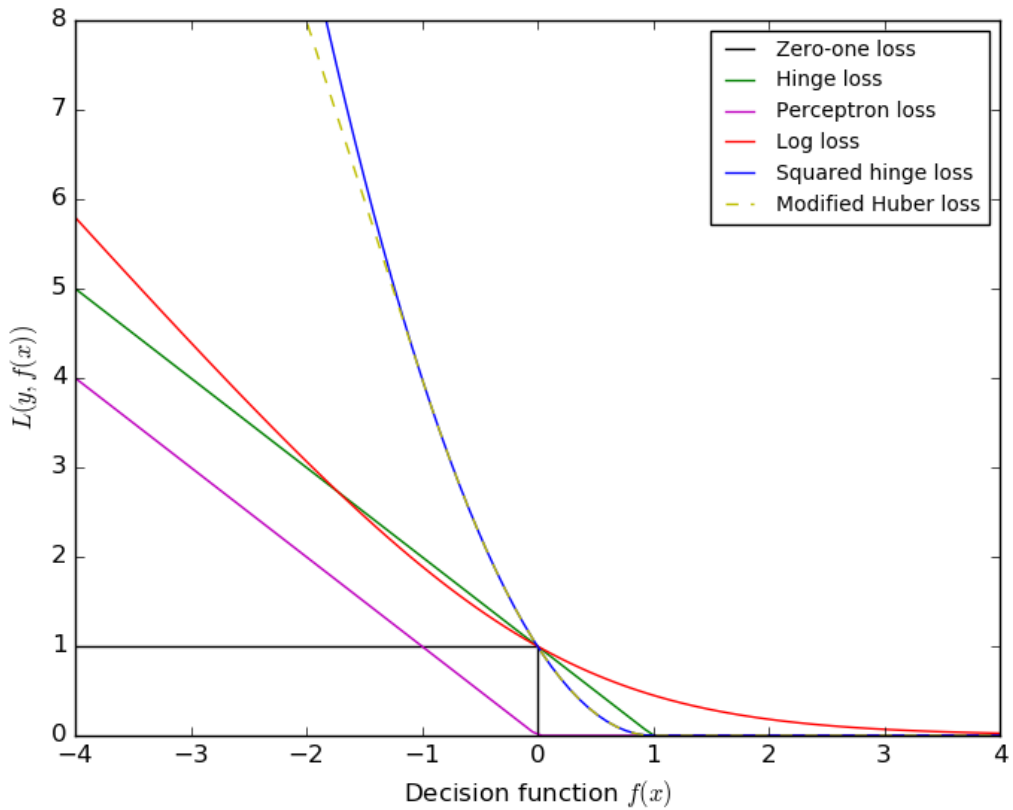
$$Y \in [-1,1] : \min_p \frac{1}{ln2}\left(1 + e^{-Yln\left(\frac{p}{1-p}\right)}\right) \qquad ln\left(\frac{p}{1-p}\right) = x^T\beta$$



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

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

$$\nabla f(\boldsymbol{a}) = \left(\frac{\partial f}{\partial x_1}(\boldsymbol{a}), \frac{\partial f}{\partial x_2}(\boldsymbol{a}), \cdots, \frac{\partial f}{\partial x_p}(\boldsymbol{a}) \right)$$

collects all the instantaneous slopes (derivatives)
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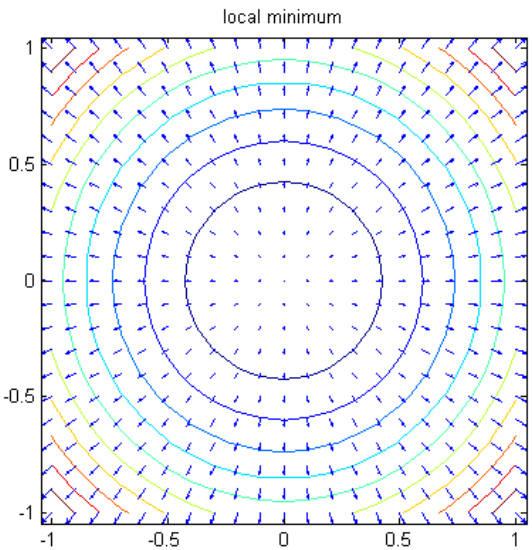

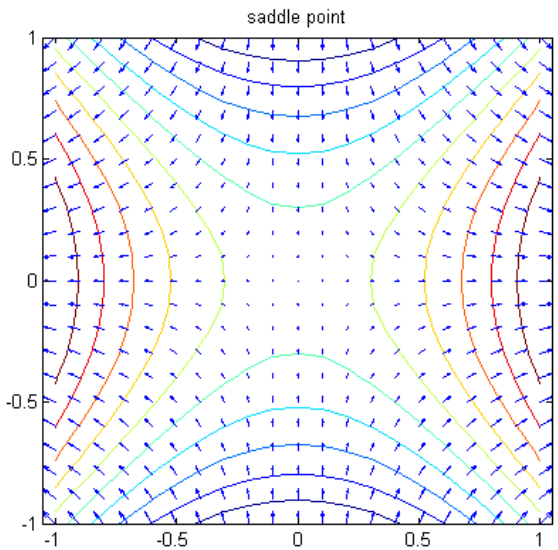

Gradient Descent

`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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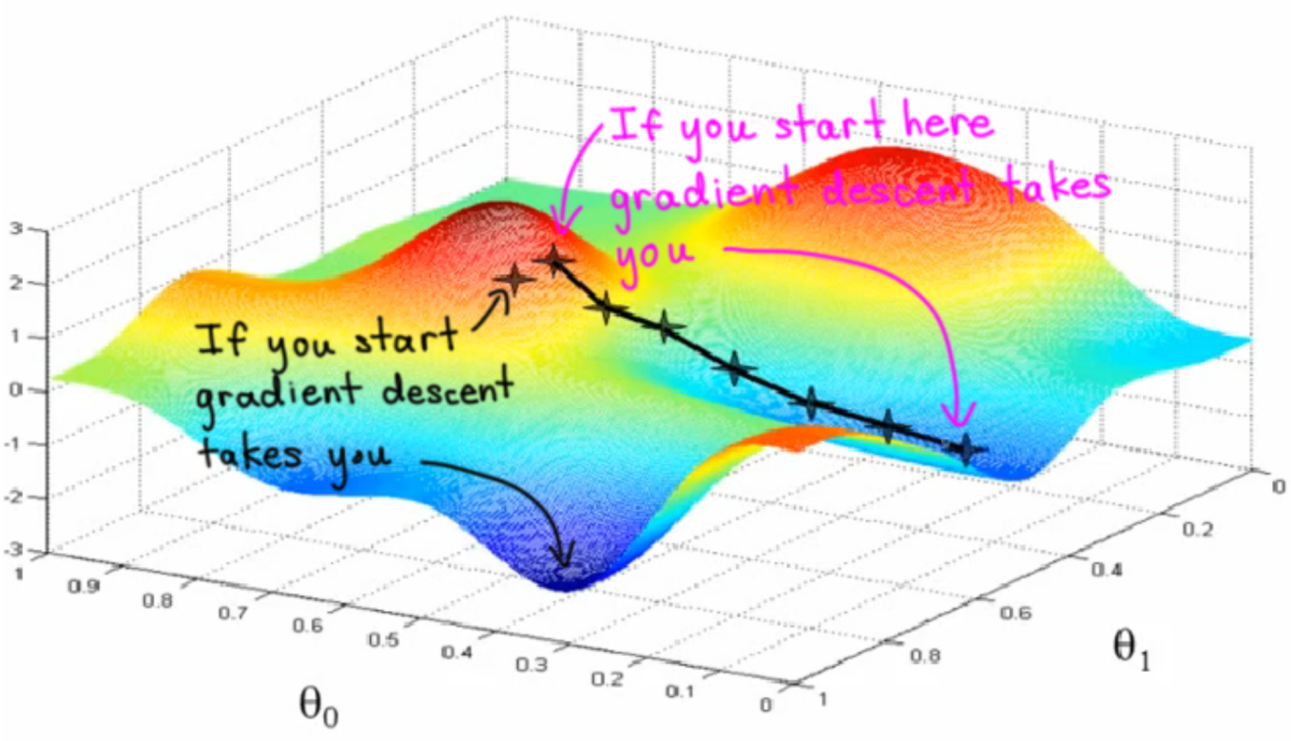
c. $|\nabla f| < \epsilon$

Pitfalls (literally)



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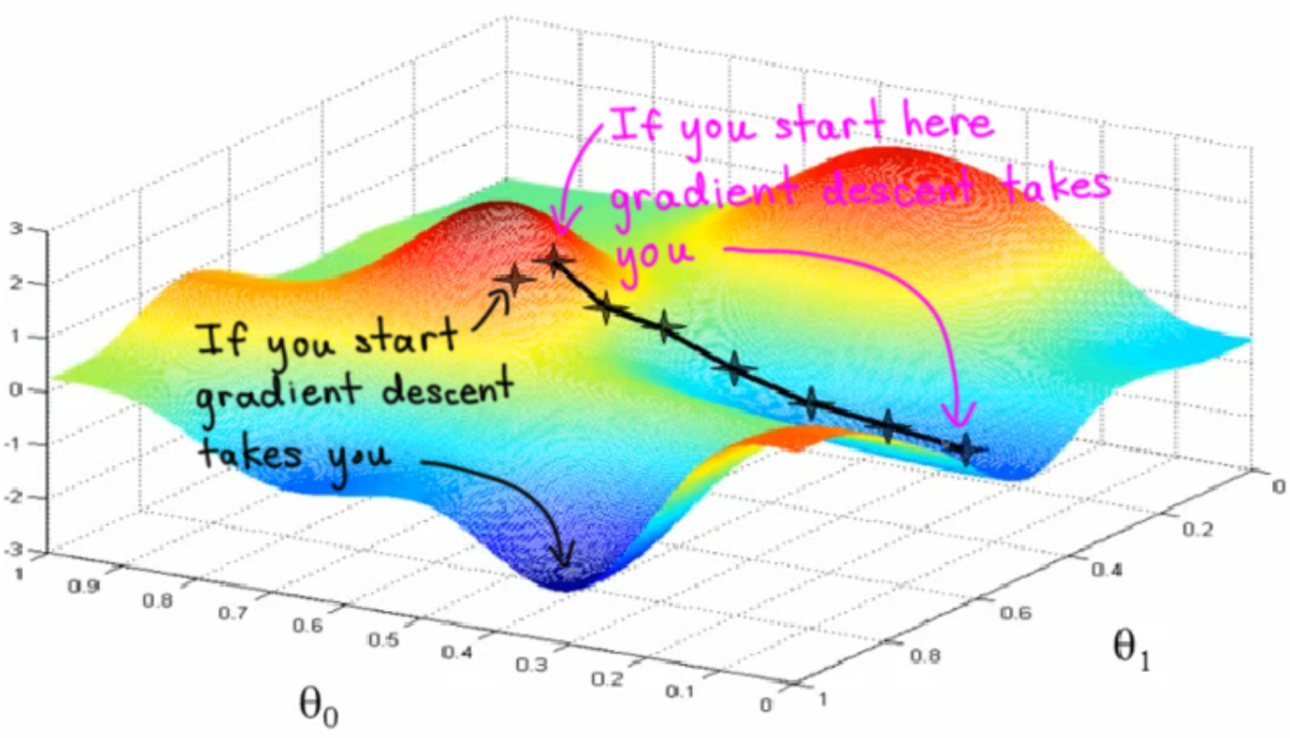
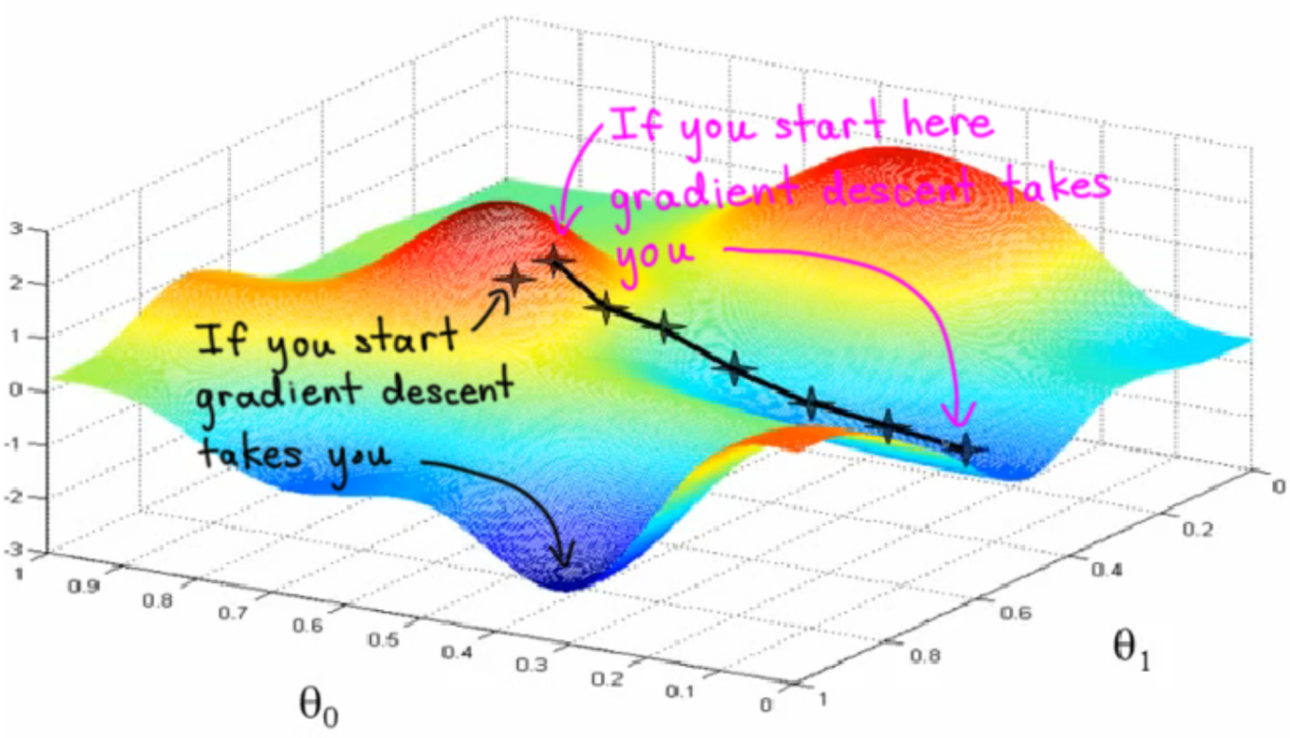


- convexity to guarantee global maximum

Pitfalls (literally)



- convexity to guarantee global maximum
- Need differentiable cost function

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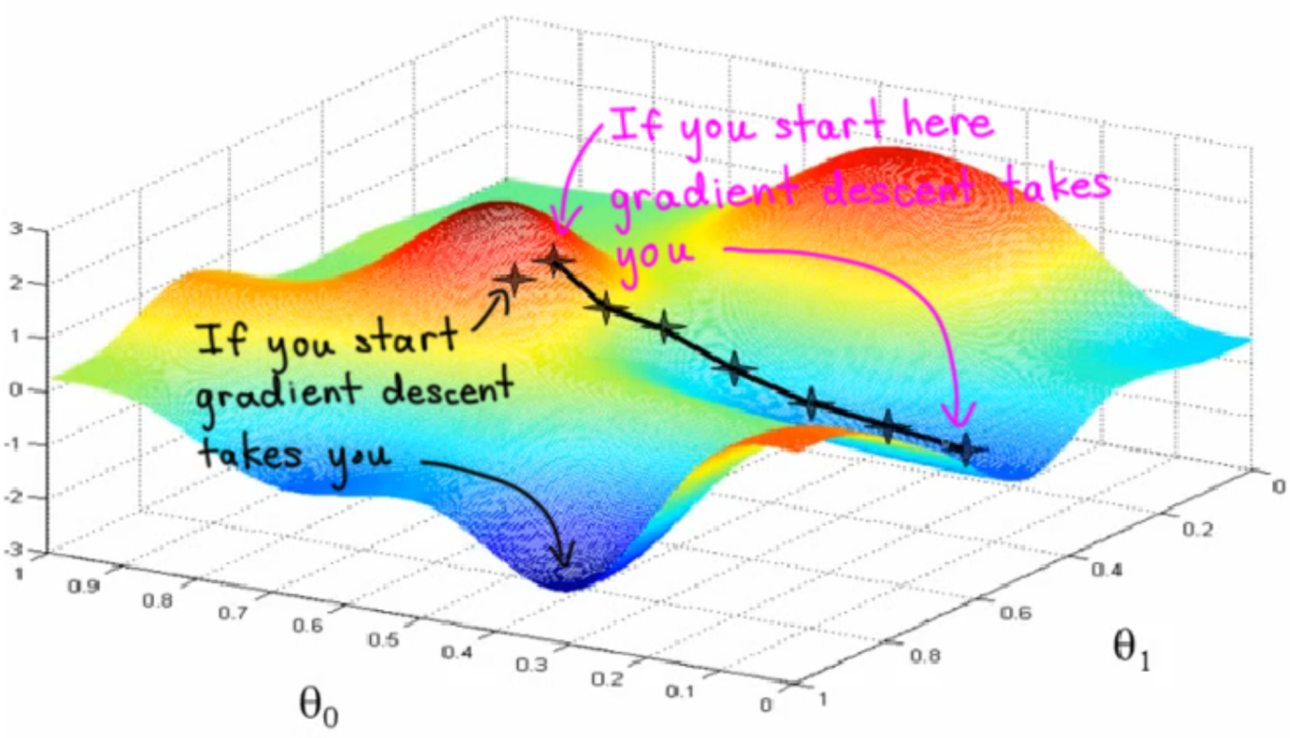

- convexity to guarantee global maximum
- Need differentiable cost function
- converges asymptotically

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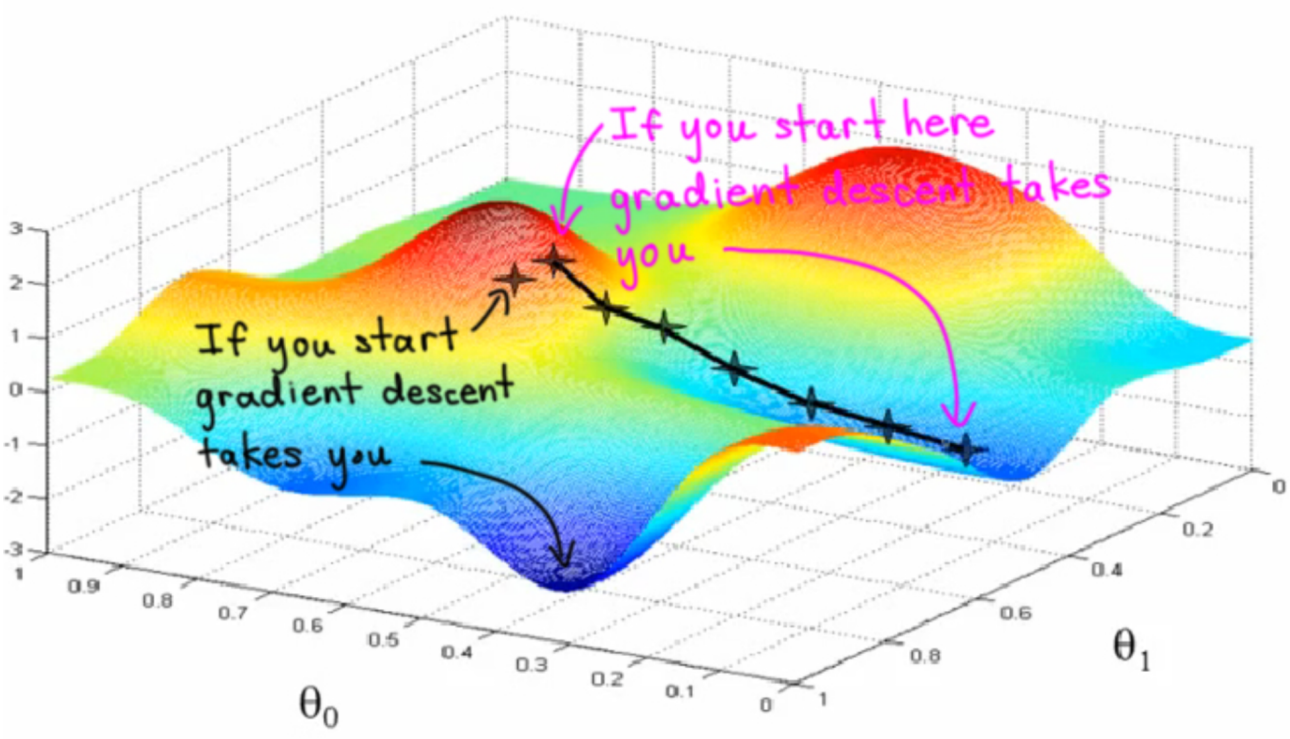
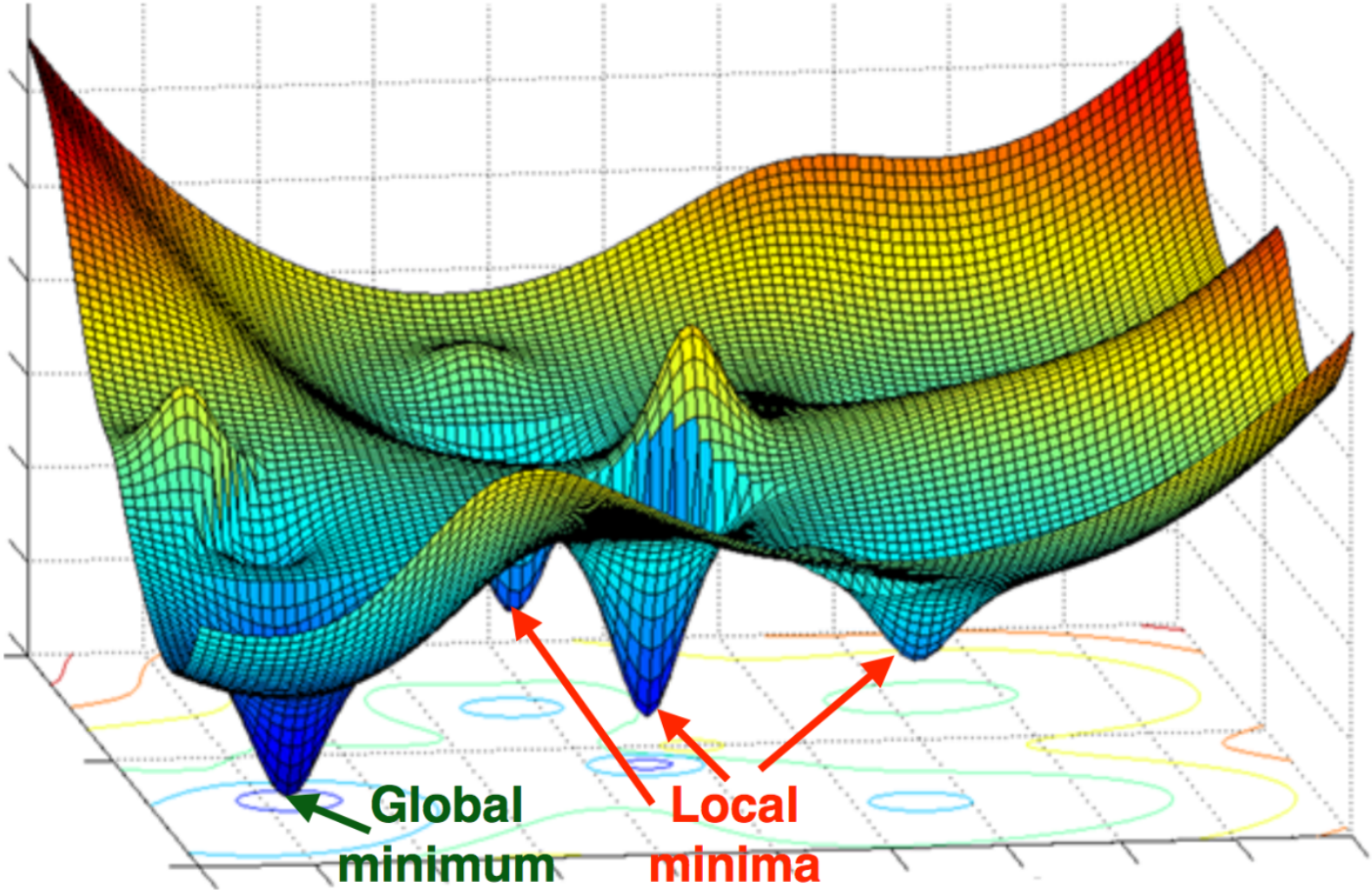


- convexity to guarantee global maximum
- Need differentiable cost function
- converges asymptotically
- good performance requires feature scaling & parameter tuning

Here's another one...



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

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

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

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

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

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

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

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

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

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

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

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

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

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It has been empirically proven to also often converge faster!

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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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2nd order information makes Newton-Raphson faster

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Inverting the Hessian matrix can be costly (or impossible)

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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

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  Depends

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  Depends
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  Probably not
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  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