Gradient Descent and such

Schwartz

July 22, 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 Descent
- Stochastic Gradient Descent
- Newton's Method

Exercise of the day

Find parameters that maximizes the fit of model to data

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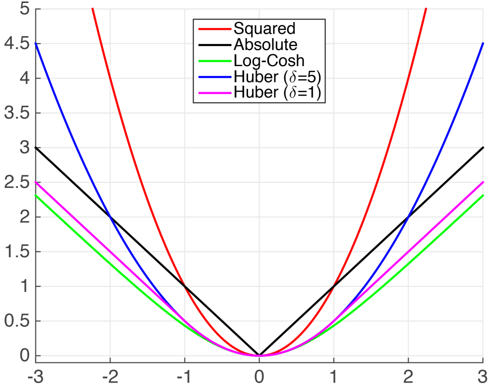
$$\hat{Y}_i \approx Y_i$$

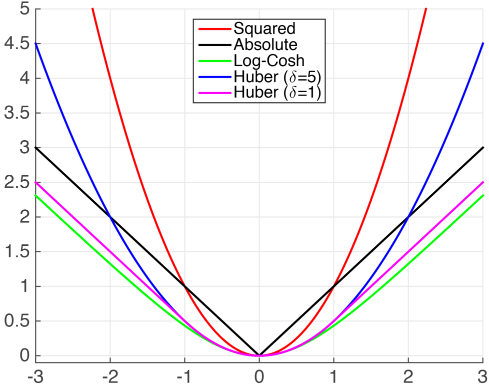
Regression Loss Functions

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



Regression Loss Functions

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



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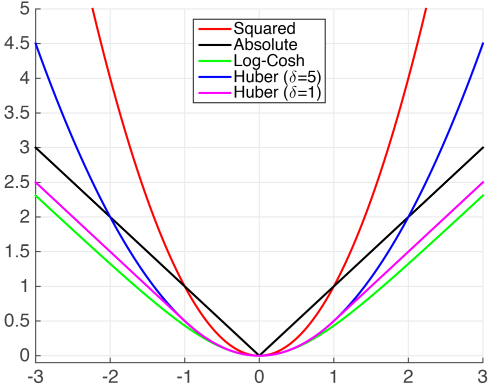
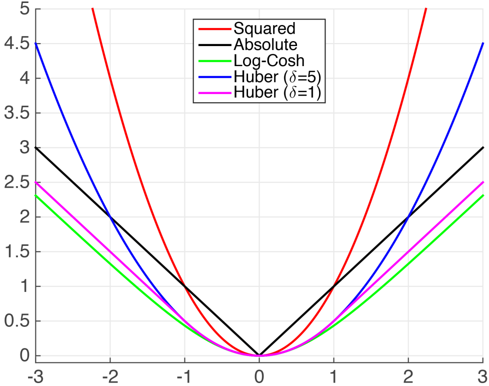


Regression Loss Functions

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

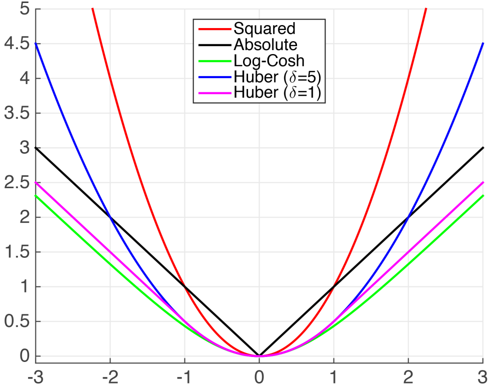
the good ol' *hyperbolic cosine* function



Regression Loss Functions

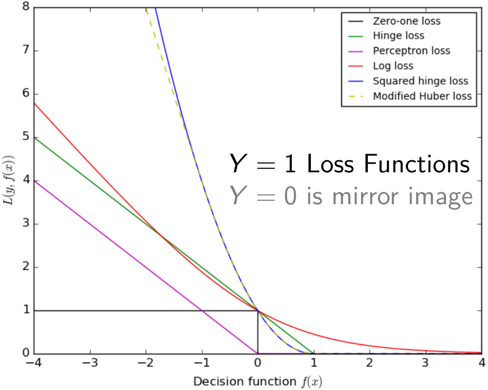
$$L_\delta(Y_i - \hat{Y}_i)$$

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



Classification Loss Functions

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



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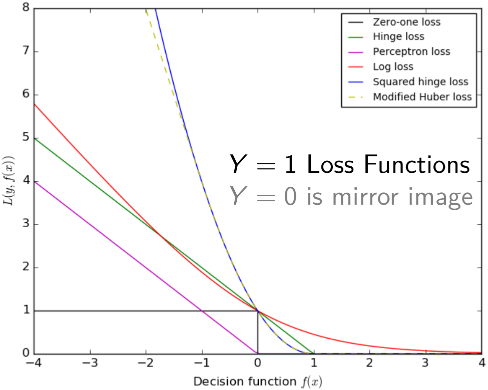

Cost function

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

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

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

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  Regularized cost functions also don't have closed form solutions

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- MLE maximizes the (log) likelihood, e.g.,

$$\underset{\beta}{argmax}\ (2\pi\sigma^2)^{-\frac{n}{2}} e^{-\frac{1}{2\sigma^2}(\mathbf{Y}-\mathbf{x}\beta)^T(\mathbf{Y}-\mathbf{x}\beta)}$$

or

$$\underset{\beta}{argmax} \prod \left(\frac{1}{1+e^{-\mathbf{x}_i^T\beta}}\right)^{Y_i} \left(\frac{1}{1+e^{\mathbf{x}_i^T\beta}}\right)^{1-Y_i}$$

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

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Gradients

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

$$\nabla_{\boldsymbol{x}} f\left(\boldsymbol{x}^{(0)}\right) = \left(\frac{\partial f}{\partial x_1}\left(\boldsymbol{x}^{(0)}\right), \frac{\partial f}{\partial x_2}\left(\boldsymbol{x}^{(0)}\right), \cdots, \frac{\partial f}{\partial x_p}\left(\boldsymbol{x}^{(0)}\right)\right)$$

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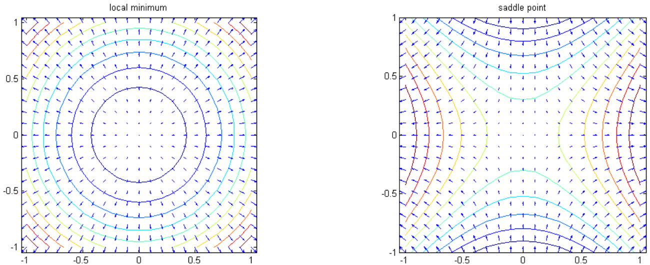

Gradient Descent

`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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Step Size α and Stopping Criterion ϵ

Here's one way to choose α:

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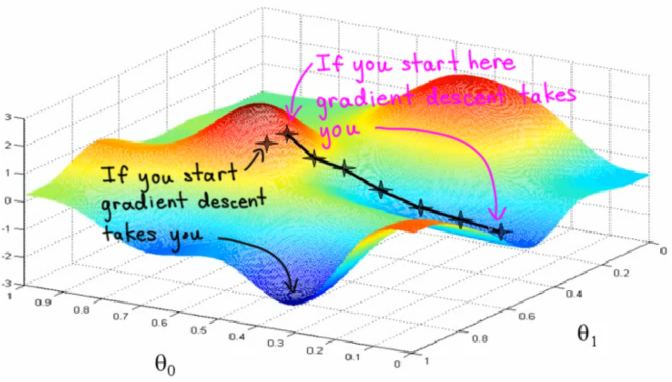
Pitfalls (literally)



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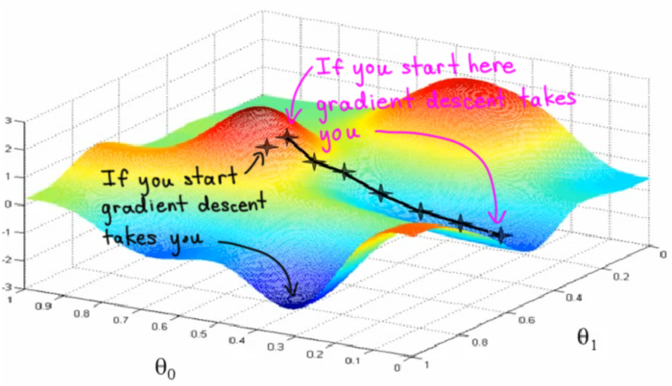

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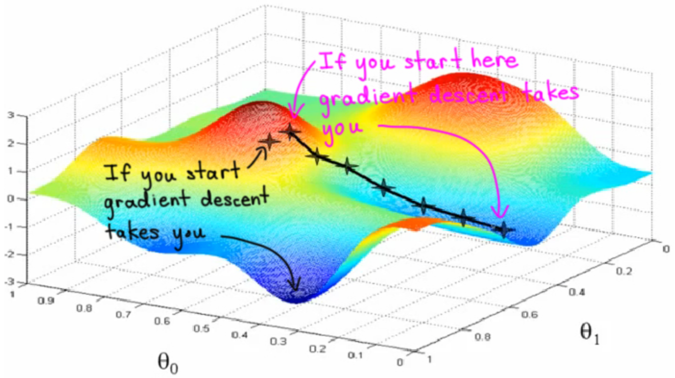

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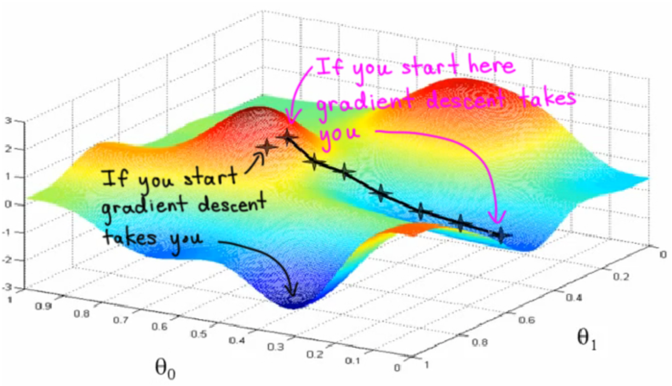

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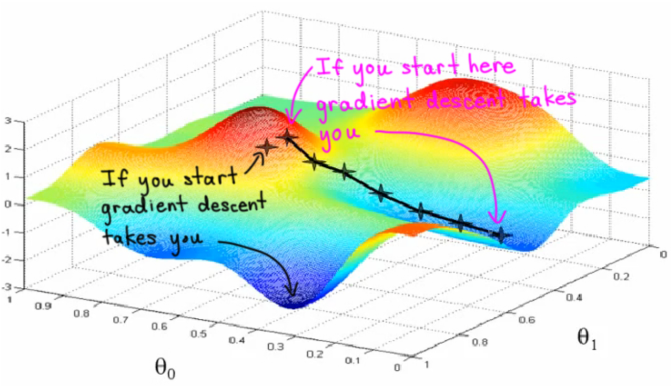
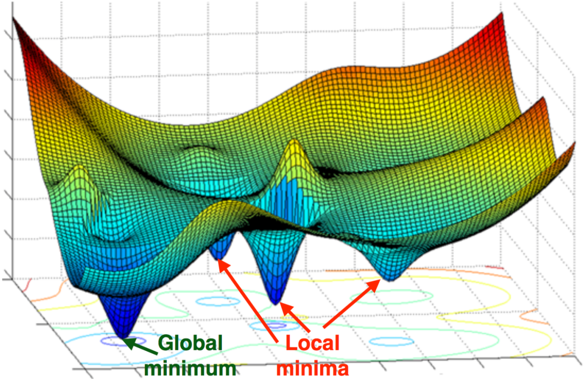
- Convergence is asymptotic...

Pitfalls (literally)



- *Convexity* required to guarantee *global minimum*
- *Differentiable cost function* required for *gradient descent*
- Convergence is asymptotic...
- Good performance requires feature scaling & parameter tuning

Pitfalls (literally)



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- *Differentiable cost function* required for *gradient descent*
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- Good performance requires feature scaling & parameter tuning

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

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First

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

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\end{aligned}$$

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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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$$\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)
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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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&= \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)
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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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Logistic regression

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

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$$\frac{\partial}{\partial\beta_j} L(\beta) \qquad -\lambda\beta$$

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

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

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$$
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\end{aligned}
$$

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

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

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

Logistic regression

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

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

$$\beta^{(t)} = \beta^{(k-1)} - \alpha\nabla\mathrm{C}(\beta^{(k-1)})$$

Potential Gradient Descent Drawbacks

1. Memory (data needs to fit)
2. Processor (cost function over all rows is expensive)

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

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It does tend to oscillate around as it nears the minimum...