UVA CS 4501: Machine Learning

Lecture 13 Extra: More about Logistic Regression

Dr. Yanjun Qi

University of Virginia

Department of
Computer Science

X_1	X_2	X_3	C

A Dataset for classification

$$f : \boxed{X} \longrightarrow \boxed{C}$$

Output as Discrete Class Label
C_1, C_2, …, C_L

Discriminative

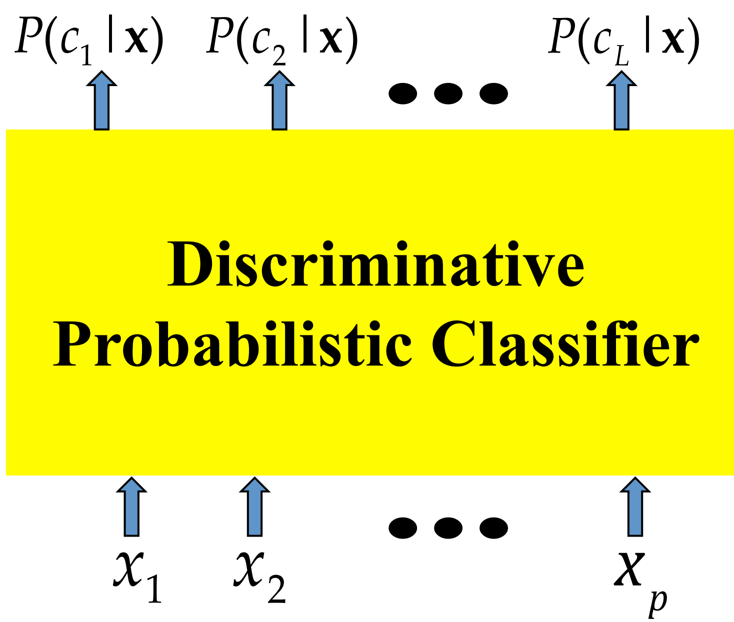
$$\boxed{\arg\max_{C} P(C/\mathbf{X}) \quad C = c_1, \cdots, c_L}$$

- **Data**/*points/instances/examples/samples/records*: [rows]
- **Features**/*attributes/dimensions/independent variables/covariates/predictors/regressors*: [columns, except the last]
- **Target**/*outcome/response/label/dependent variable*: special column to be predicted [last column]

Establishing a probabilistic model for classification

– **Discriminative model**

$$\hat{c} = \arg\max_{C} P(C / \mathbf{X}), \quad C = c_1, \cdots, c_L$$



$$\mathbf{x} = (x_1, x_2, \cdots, x_p)$$

Adapt from Prof. Ke Chen NB slides

A Dataset for classification

X_1	X_2	X_3	C

$$f : \boxed{X} \longrightarrow \boxed{C}$$

Output as Discrete Class Label $C_1, C_2, \ldots, C_L$

Discriminative $\rightarrow$ $$\arg\max_{C} P(C/\mathbf{X}) \quad C = c_1, \cdots, c_L$$

Generative $\rightarrow$ $$\operatorname*{argmax}_{C} P(C|X) = \operatorname*{argmax}_{C} P(X,C) = \operatorname*{argmax}_{C} P(X|C)P(C)$$

Later!

- **Data**/*points/instances/examples/samples/records*: [rows]
- **Features**/*attributes/dimensions/independent variables/covariates/predictors/regressors*: [columns, except the last]
- **Target**/*outcome/response/label/dependent variable*: special column to be predicted [last column]

Today: Extra

- ✓ Bayes Classifier and MAP Rule?
  - Bayes Classifier
  - Empirical Prediction Error
  - 0-1 Loss function for Bayes Classifier

- ✓ Logistic regression
  - Parameter Estimation for LR

$$p(y|x) = \frac{e^{\beta x}}{1+e^{\beta x}}$$

$$\Downarrow$$

$$\vec{\beta}$$

Bayes classifiers

- Treat each feature attribute and the class label as random variables.

Bayes classifiers

- Treat each feature attribute and the class label as random variables.

- Given a sample **x** with attributes ($x_1, x_2, \ldots, x_p$):
  - Goal is to predict its class *C*.
  - Specifically, we want to find the value of C_i that maximizes $p(C_i \mid x_1, x_2, \ldots, x_p)$.

Bayes classifiers

- Treat each feature attribute and the class label as random variables.

- Given a sample **x** with attributes ($x_1, x_2, \ldots, x_p$):
  - Goal is to predict its class *C*. $\rightarrow \{C_1, C_2, \ldots, C_L\}$
  - Specifically, we want to find the value of C_i that maximizes $p(C_i \mid x_1, x_2, \ldots, x_p)$.

- Can we estimate $p(C_i \mid \mathbf{x}) = p(C_i \mid x_1, x_2, \ldots, x_p)$ directly from data?

Bayes classifiers → MAP classification rule

- Establishing a probabilistic model for classification

→ **MAP** classification rule

– **MAP**: **M**aximum **A** **P**osterior

Bayes classifiers
➔ MAP classification rule

- Establishing a probabilistic model for classification

➔ **MAP** classification rule

- **MAP**: **M**aximum **A** **P**osterior
- Assign x to c^* if

$$P(C = c^* \mid \mathbf{X} = \mathbf{x}) > P(C = c \mid \mathbf{X} = \mathbf{x})$$

$$\text{for } c \neq c^*, \ c = c_1, \cdots, c_L$$

Adapt from Prof. Ke Chen NB slides

Bayes classifiers
→ MAP classification rule

- Establishing a probabilistic model for classification

→ **MAP** classification rule

- **MAP**: **M**aximum **A** **P**osterior
- Assign x to c^* if

$$\boxed{P(C=c^* \mid \mathbf{X}=\mathbf{x}) > P(C=c \mid \mathbf{X}=\mathbf{x})} \quad c \neq c^*,\ c = c_1, \cdots, c_L$$

$$\left.\begin{cases} P(C=C_1 \mid x) \\ P(C=C_2 \mid x) \\ P(C=C_3 \mid x) \end{cases}\right\} \max \Rightarrow C_i$$

Adapt from Prof. Ke Chen NB slides

Bayes Classifiers – MAP Rule

Task: Classify a new instance *X* based on a tuple of attribute values $X = \langle X_1, X_2, \ldots, X_p \rangle$ into one of the classes

$$c_{MAP} = \underset{c_j \in C}{\operatorname{argmax}} P(c_j \mid x_1, x_2, \ldots, x_p)$$

WHY ?

MAP = Maximum Aposteriori Probability

Adapt From Carols' prob tutorial

0-1 LOSS for Classification

- Procedure for categorical output variable C

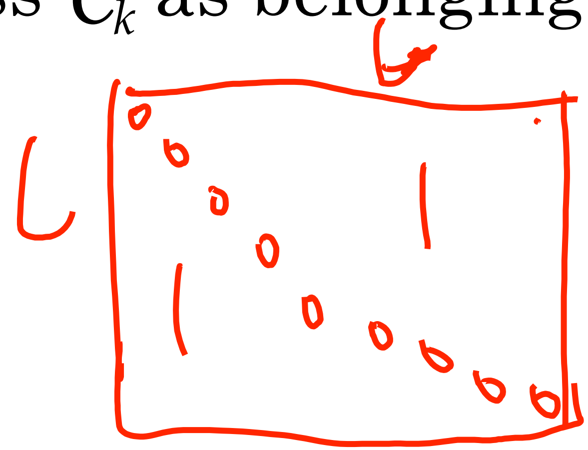
if $k=\ell$, $L(k,\ell)=0$

- Frequently, 0-1 loss function used: $\boxed{L(k, \ell)}$

if $k \neq \ell$, $L(k,\ell)=1$

- $L(k, \ell)$ is the price paid for misclassifying an element from class C_k as belonging to class C_ℓ

➔ *L*L matrix*



$C_1, C_2, \cdots, C_L$

Expected prediction error (EPE)

- Expected prediction error (EPE), with expectation taken w.r.t. the joint distribution Pr(C,X)
  - $\Pr(C,X)=\Pr(C \mid X)\Pr(X)$

e.g. 0-1 loss

$E_x(X)$

$E_x(g(x))$

$$\mathrm{EPE}(f)=E_{X,C}(L(C,f(X)))$$

$$=\mathrm{E}_X\sum_{k=1}^{L}L[C_k,f(X)]\Pr(C_k \mid X)$$

Consider sample population distribution

$$EPE(f) = E_{X,C}\left(L(C, f(X))\right)$$

$$E_C(C) = \sum_{i=1}^{L} C_i \, p(C_i)$$

$$= E_X \underbrace{E_{C|X}}_{\text{Discrete RV's Expectation}} \left[L(C, f(X)) \,\middle|\, X \right]$$

$$= E_X \sum_{k=1}^{L} L[C_k, f(X)] \, Pr(C_k | X)$$

$$\arg\min_f EPE(f(X))$$

$\Rightarrow$ Pointwise minization when $X = x$

$$\Rightarrow \hat{f}(X = x) = \arg\min_{f(x) \in C} \sum_{k=1}^{L} \underbrace{L[C_k, f(x)]}_{\begin{bmatrix} 0 & & 1 \\ & 0 & \\ 1 & & 0 \end{bmatrix}_{L \times L}} Pr(C_k | X = x)$$

$$\Rightarrow \hat{f}(x) = \arg\max_{C_k \in \{C_1, C_2, C_3, \ldots, C_L\}} Pr(C_k | X = x)$$

$$\left\{ \begin{array}{l} p(C_1 | x) \\ p(C_2 | x) \\ \vdots \\ p(C_L | x) \end{array} \right.$$

Expected prediction error (EPE)

$$\mathrm{EPE}(f) = E_{X,C}(L(C,f(X)) = \mathrm{E}_X \sum_{k=1}^{K} L[C_k, f(X)]\Pr(C_k \mid X)$$

Consider sample population distribution

- Pointwise minimization suffices

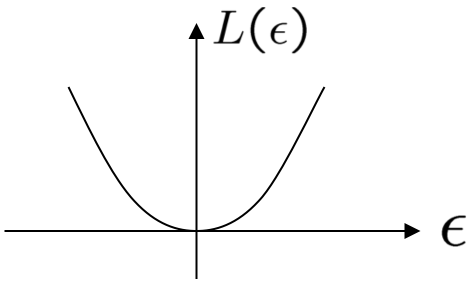
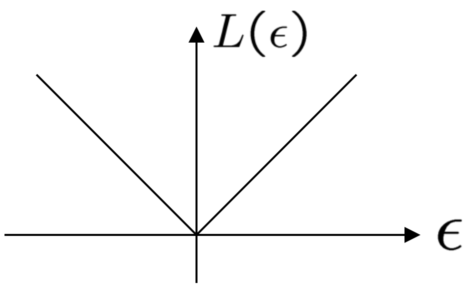
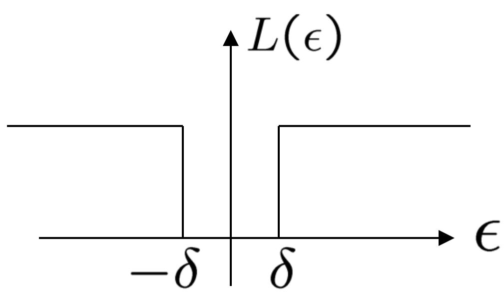
- ➔ simply $$\hat{f}(X) = \mathrm{argmin}_{g \in C} \sum_{k=1}^{K} L(C_k, g)\Pr(C_k \mid X = x)$$

$$\hat{f}(X) = C_k \text{ if}$$

$$\Pr(C_k \mid X = x) = \max_{g \in C} \Pr(g \mid X = x)$$

Bayes Classifier

SUMMARY: WHEN EPE USES DIFFERENT LOSS

	Loss Function	Estimator $\hat{f}(x)$
L_2		$EPE = E_{X,Y}(Y - f(x))^2$ $\hat{f}(x) = E[Y \mid X = x]$
L_1		$\hat{f}(x) = \text{median}(Y \mid X = x)$
0-1		$\hat{f}(x) = \arg\max_Y P(Y \mid X = x)$ (Bayes classifier / MAP)

Today: Extra

- ✓ Why Bayes Classification – MAP Rule?
  - Empirical Prediction Error
  - 0-1 Loss function for Bayes Classifier

- ✓ Logistic regression
  - Parameter Estimation for LR

$$p(y|x) = \frac{e^{\beta x}}{1+e^{\beta x}}$$

$$\Downarrow$$

$$\vec{\beta}$$

Newton's method for optimization

- The most basic second-order optimization algorithm
- Updating parameter with

GD: $\theta_{k+1} = \theta_k - \alpha g_k$

Newton: $$\theta_{k+1} = \theta_k - \underbrace{\mathbf{H}_K^{-1} \mathbf{g}_k}_{p \times 1}$$

$p \times p$ $\quad$ $p \times 1$

Review: Hessian Matrix / n==2 case

Singlevariate → multivariate

$$f(x,y)$$

- 1^{st} derivative to gradient,

$$g = \nabla f = \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{pmatrix}$$

- 2^{nd} derivative to Hessian

$$H = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix}$$

Review: Hessian Matrix

Suppose that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a function that takes a vector in $\mathbb{R}^n$ and returns a real number. Then the ***Hessian*** matrix with respect to x, written $\nabla_x^2 f(x)$ or simply as H is the $n \times n$ matrix of partial derivatives,

$$\nabla_x^2 f(x) \in \mathbb{R}^{n \times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}.$$

Newton's method for optimization

- Making a quadratic/second-order Taylor series approximation

$$\hat{f}_{quad}(\boldsymbol{\theta}) = f(\boldsymbol{\theta}_k) + \mathbf{g}_k^T(\boldsymbol{\theta} - \boldsymbol{\theta}_k) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_k)^T\mathbf{H}_k(\boldsymbol{\theta} - \boldsymbol{\theta}_k)$$

Finding the minimum solution of the above right quadratic approximation (quadratic function minimization is easy !)

$$\hat{f}(\theta) = f(\theta_k) + g_k^T(\theta - \theta_k) + \underbrace{\frac{1}{2}(\theta-\theta_k)^T H_k (\theta - \theta_k)}$$

$$\Downarrow$$

$$\frac{1}{2}\left(\theta^T H_k \theta - 2\theta^T H_k \theta_k + \theta_k^T H_k \theta_k\right)$$

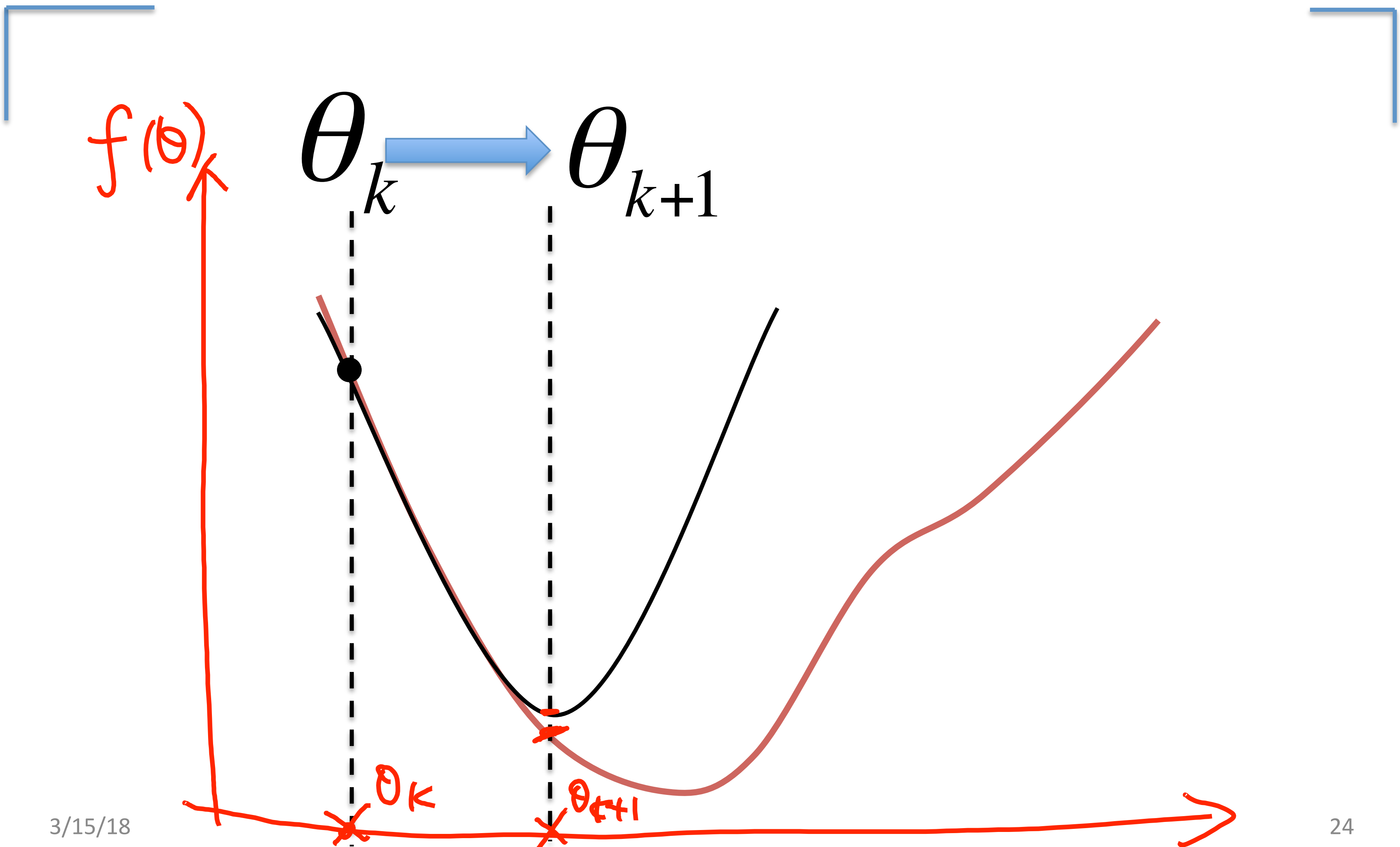
$$\frac{\partial \hat{f}(\theta)}{\partial \theta} = 0 + g_k + \underbrace{\frac{2}{2} H_k \theta - \frac{2}{2} H_k \theta_k}_{\text{see p24 handout}} := 0$$

$$g_k + H_k(\theta - \theta_k) = 0$$

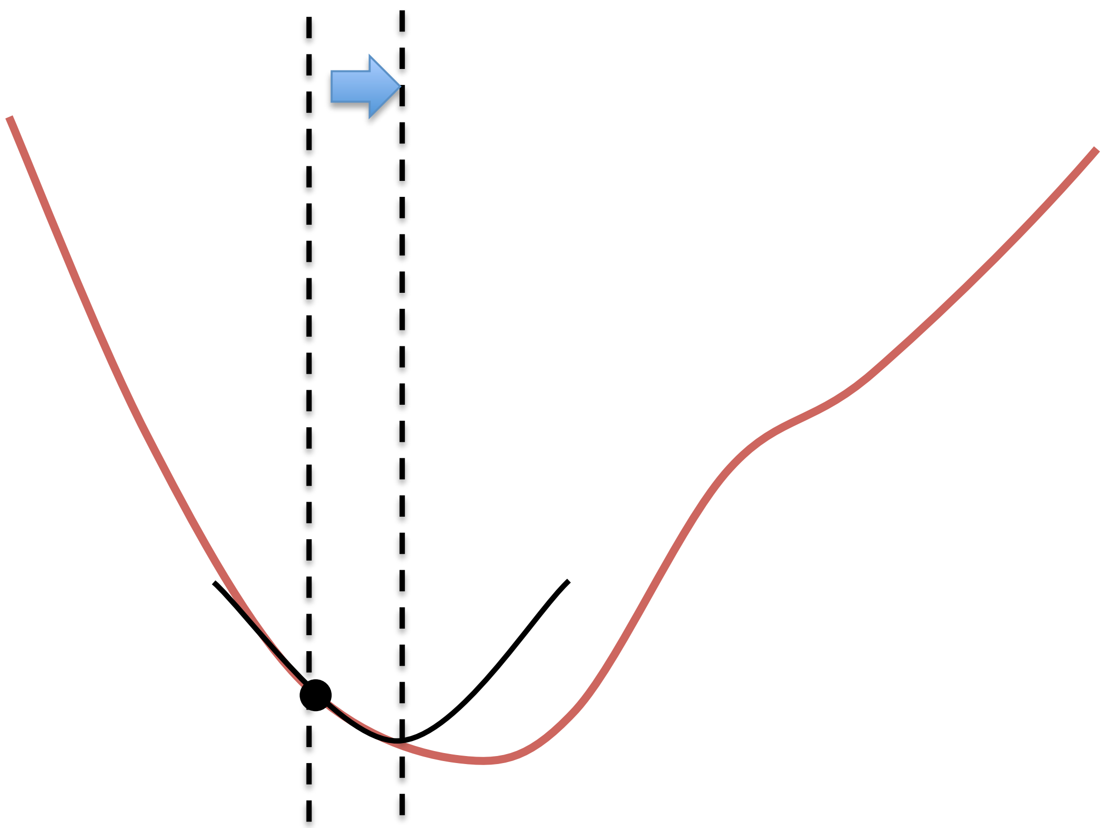
$$\Rightarrow \quad \theta = \theta_k - H_k^{-1} g_k$$

where $\begin{cases} H_k \in R^{p \times p} \\ g_k \in R^p \end{cases}$

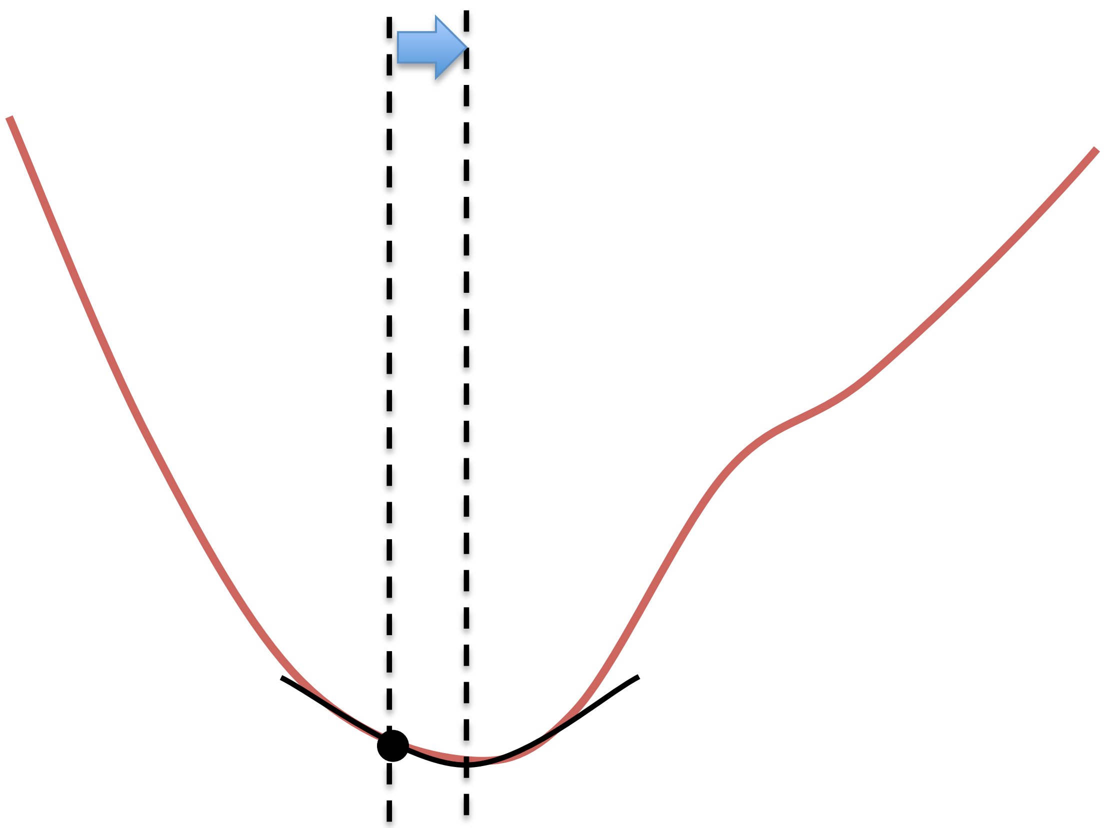
Newton's Method / second-order Taylor series approximation



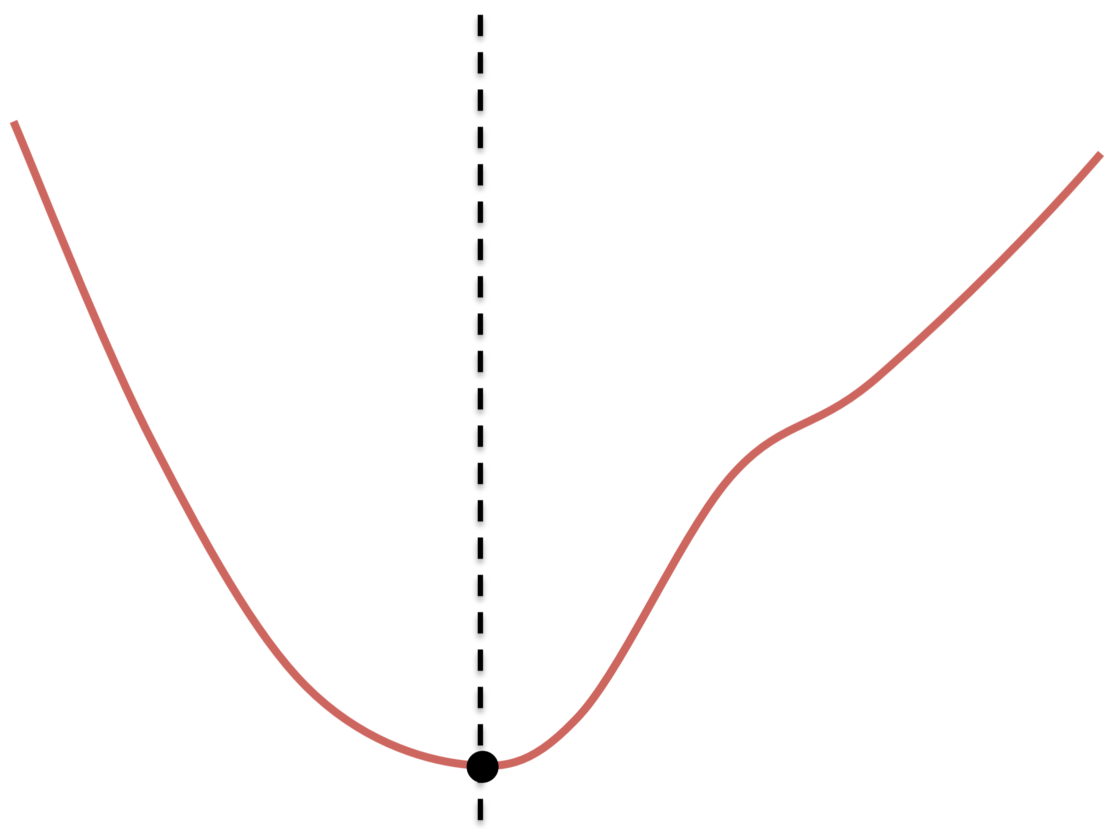
Newton's Method / second-order Taylor series approximation



Newton's Method / second-order Taylor series approximation



Newton's Method / second-order Taylor series approximation



Newton's Method

- At each step:

$$\theta_{k+1} = \theta_k - \frac{f'(\theta_k)}{f''(\theta_k)}$$

$$\theta_{k+1} = \theta_k - H^{-1}(\theta_k)\nabla f(\theta_k)$$

- Requires 1st and 2nd derivatives
- Quadratic convergence
- → However, finding the inverse of the Hessian matrix is often expensive

Newton vs. GD for optimization

- Newton: a quadratic/second-order Taylor series approximation

$$\theta_{k+1} = \theta_k - \frac{1}{H(\theta_k)} g(\theta_k)$$

$$\hat{f}_{quad}(\boldsymbol{\theta}) = f(\boldsymbol{\theta}_k) + \mathbf{g}_k^T(\boldsymbol{\theta} - \boldsymbol{\theta}_k) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_k)^T \mathbf{H}_k (\boldsymbol{\theta} - \boldsymbol{\theta}_k)$$

Finding the minimum solution of the above right quadratic approximation (quadratic function minimization is easy !)

- GD: a approximation

$$\hat{f}_{quad}(\boldsymbol{\theta}) = f(\boldsymbol{\theta}_k) + \mathbf{g}_k^T(\boldsymbol{\theta} - \boldsymbol{\theta}_k) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_k)^T \frac{1}{\alpha} (\boldsymbol{\theta} - \boldsymbol{\theta}_k)$$

$$\Downarrow$$

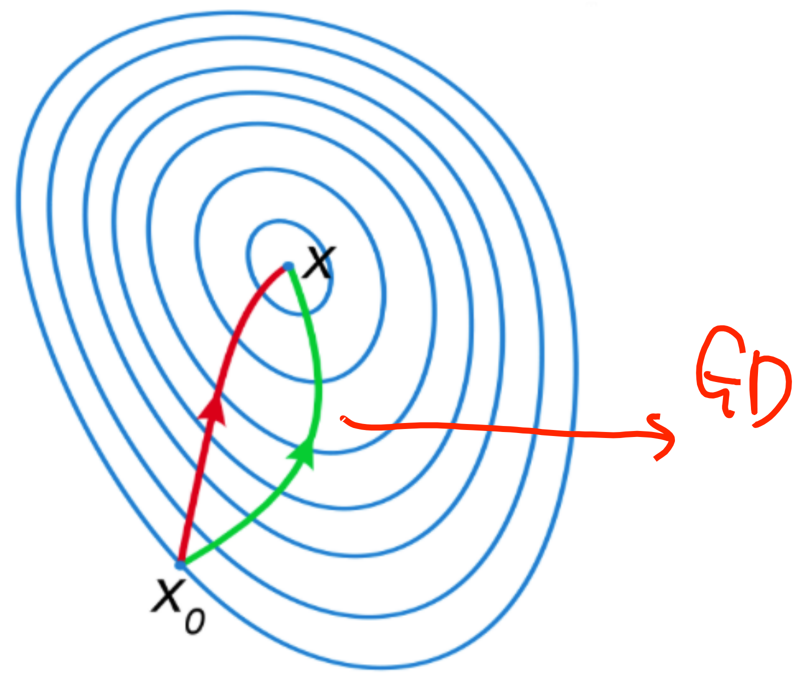
$$\theta_{k+1} = \theta_k - \alpha\, g(\theta_k)$$

Comparison

- Newton’s method vs. Gradient descent

A comparison of gradient descent (green) and Newton's method (red) for minimizing a function (with small step sizes).

Newton’s method uses curvature information to get a more direct route ...



Parameter Estimation for LR → MLE from the data

- RECAP: Linear regression → Least squares

- Logistic regression: → Maximum likelihood estimation

MLE for Logistic Regression Training

Let's fit the logistic regression model for K=2, i.e., number of classes is 2

For Bernoulli distribution

$$p(y|x)^y(1-p)^{1-y}$$

Training set: (x_i, y_i), i=1,…,N

(conditional) Log-likelihood:

How?

$$l(\beta)=\sum_{i=1}^{N}\{\log\Pr(Y=y_i|X=x_i)\}$$

$$=\sum_{i=1}^{N}y_i\log(\Pr(Y=1|X=x_i))+(1-y_i)\log(\Pr(Y=0|X=x_i))$$

$$=\sum_{i=1}^{N}(y_i\log\frac{\exp(\beta^Tx_i)}{1+\exp(\beta^Tx_i)})+(1-y_i)\log\frac{1}{1+\exp(\beta^Tx_i)})$$

$$=\sum_{i=1}^{N}(y_i\beta^Tx_i-\log(1+\exp(\beta^Tx_i)))$$

x_i are (p+1)-dimensional input vector with leading entry 1
\beta is a (p+1)-dimensional vector

We want to maximize the log-likelihood in order to estimate *\beta*

$$l(\beta)=\sum_{i=1}^{N}\{\log \Pr(Y=y_i \mid X=x_i)\}$$

y_i

$\log\{\Pr(Y=y_i \mid X=x_i) = p(y_i \mid x_i)\} \Rightarrow$ $y_i=1$ $\rightarrow p(y_i=1 \mid x)$; $y_i=0$ $\rightarrow 1-p(y_i=1 \mid x)$

$= \log\{p(y_i=1 \mid x)^{y_i}(1-p(y_i=1 \mid x_i))^{1-y_i}\}$

$= y_i \log p(y_i=1 \mid x) + (1-y_i)\log(1-p(y_i=1 \mid x))$

Newton-Raphson for LR (optional)

$$\frac{\partial l(\beta)}{\partial \beta} = \sum_{i=1}^{N} (y_i - \frac{\exp(\beta^T x)}{1+\exp(\beta^T x)}) x_i = 0$$

Vector

(*p*+1) Non-linear equations to solve for (*p*+1) unknowns β

Solve by Newton-Raphson method:

$$\beta^{new} \leftarrow \beta^{old} - [(\frac{\partial^2 l(\beta)}{\partial \beta \partial \beta^T})]^{-1} \frac{\partial l(\beta)}{\partial \beta},$$

$$\text{where, } (\frac{\partial^2 l(\beta)}{\partial \beta \partial \beta^T}) = -\sum_{i=1}^{N} x_i x_i^T (\frac{\exp(\beta^T x_i)}{1+\exp(\beta^T x_i)})(\frac{1}{1+\exp(\beta^T x_i)})$$

$p(x_i ; \beta)$

$1 - p(x_i ; \beta)$

minimizes a quadratic approximation
to the function we are really interested in.

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \mathbf{H}_K^{-1} \mathbf{g}_k$$

Newton-Raphson for LR…

$$\frac{\partial l(\beta)}{\partial \beta} = \sum_{i=1}^{N} (y_i - \frac{\exp(\beta^T x)}{1+\exp(\beta^T x)}) x_i = X^T (y-p)$$

$p(y=1|x) = \frac{e^{\beta x}}{1+e^{\beta x}}$

$$(\frac{\partial^2 l(\beta)}{\partial \beta \partial \beta^T}) = -X^T W X$$

So, NR rule becomes: $\beta^{new} \leftarrow \beta^{old} + (X^T W X)^{-1} X^T (y-p),$

$$X = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{bmatrix}_{N-by-(p+1)}, \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}_{N-by-1}, \quad p = \begin{bmatrix} \exp(\beta^T x_1)/(1+\exp(\beta^T x_1)) \\ \exp(\beta^T x_2)/(1+\exp(\beta^T x_2)) \\ \vdots \\ \exp(\beta^T x_N)/(1+\exp(\beta^T x_N)) \end{bmatrix}_{N-by-1},$$

$X : N\times(p+1)$ matrix of x_i

$y : N\times 1$ matrix of y_i

$p : N\times 1$ matrix of $p(x_i;\beta^{old})$

$W : N\times N$ diagonal matrix of $p(x_i;\beta^{old})(1-p(x_i;\beta^{old}))$

$$(\frac{\exp(\beta^T x_i)}{(1+\exp(\beta^T x_i))})(1-\frac{1}{(1+\exp(\beta^T x_i))})$$

Newton-Raphson for LR…

1

- Newton-Raphson
  - $\beta^{new} = \beta^{old} + (X^T W X)^{-1} X^T (y-p)$

    $= (X^T W X)^{-1} X^T W (X\beta^{old} + W^{-1}(y-p))$

    $= (X^T W X)^{-1} X^T W z$

    $(X^T X)^{-1} X^T Y$

    W

    Wz

    Re expressing Newton step as weighted least square step
  - Adjusted response

    $z = X\beta^{old} + W^{-1}(y-p)$
  - Iteratively reweighted least squares (IRLS)

    $\beta^{new} \leftarrow \arg\min_{\beta} (z - X\beta^T)^T W (z - X\beta^T)$

    $\leftarrow \arg\min_{\beta} (y-p)^T W^{-1} (y-p)$

References

- Prof. Tan, Steinbach, Kumar's "Introduction to Data Mining" slide
- Prof. Andrew Moore's slides
- Prof. Eric Xing's slides
- Prof. Ke Chen NB slides
- Hastie, Trevor, et al. *The elements of statistical learning*. Vol. 2. No. 1. New York: Springer, 2009.