

Mathematical Preliminaries

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2008.9.17



Outline

- Linear Algebra
- Concepts from Geometry
- Elements of Differential Calculus



Data Fitting

- Examples

- Find the least-squares solution \vec{x}^* of the system $A\vec{x} = \vec{b}$, where

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \text{ and } \vec{b} = \begin{bmatrix} 0 \\ 0 \\ 6 \end{bmatrix}$$

- Fit a quadratic function to the four data points $(a_1, b_1) = (-1, 8)$, $(a_2, b_2) = (0, 8)$, $(a_3, b_3) = (1, 4)$, and $(a_4, b_4) = (2, 16)$.

Data Fitting

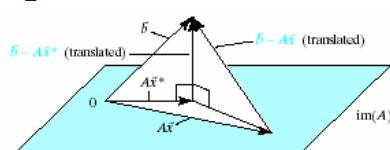
- Given data points $(a_1, b_1), (a_2, b_2), \dots, (a_n, b_n)$

- L_2 regression (QP): $\arg \max_{\mathbf{x}} \sum_j (b_j - \mathbf{x}a_j)^2$

- L_1 regression: $\arg \max_{\mathbf{x}} \sum_j \|b_j - \mathbf{x}a_j\|$

- Least-square regression (L_2)

$$\|\vec{b} - A\vec{x}^*\| \leq \|\vec{b} - A\vec{x}\|$$





Quadratic Form

- Example

- Consider the quadratic form

$$q(x_1, x_2, x_3) = 9x_1^2 + 7x_2^2 + 3x_3^2 - 2x_1x_2 + 4x_1x_3 - 6x_2x_3.$$

Find a symmetric matrix A such that $q(\vec{x}) = \vec{x} \cdot A\vec{x}$ for all \vec{x} in \mathbb{R}^3 .

- Matrix form $q(\mathbf{x}) = \mathbf{x}^T Q \mathbf{x}$



Hyperplanes

- Hyperplane

- $H = \{x \in \mathbb{R}^n \mid u_1x_1 + u_2x_2 + \dots + u_nx_n = u^T x = v\}$
- $a \in H, H = \{x \in \mathbb{R}^n \mid u^T(x-a)=0\}$

- Halfspace

- $H_+ = \{x \in \mathbb{R}^n \mid u^T x \geq v\}$
- $H_- = \{x \in \mathbb{R}^n \mid u^T x \leq v\}$

Convex Set

- Line segment
 - $x, y \in \mathbb{R}^n, \{ v \mid v = \alpha x + (1-\alpha)y, \alpha \in [0,1] \}$
- Convex set
 - A set Θ is convex if, for all $x, y \in \Theta$, the line segment between x and y lies in Θ .



Polytopes and Polyhedra

- Convex polytope
 - A set that can be expressed as the intersection of a finite number of half-spaces
- Polyhedron
 - A nonempty bounded polytope





Differential calculus

- Consider a function $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$
- Affine function
 - A function $A: \mathbb{R}^n \rightarrow \mathbb{R}^m$ is affine if there exists a linear function $L: \mathbb{R}^n \rightarrow \mathbb{R}^m$ and a vector $y \in \mathbb{R}^m$ such that $A(x) = L(x) + y$.
 - In $\mathbb{R} \rightarrow \mathbb{R}$, an affine function has the form $A(x) = ax + b$, with $a, b \in \mathbb{R}$.
- Idea: Approximating an arbitrary function $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ near point x_0 by an affine function L .

$$\begin{aligned} A(x_0) &= f(x_0) & f(x_0) &= A(x_0) = L(x_0) + y \\ A(x) &= L(x - x_0) + f(x_0) & y &= f(x_0) - L(x_0) \\ \lim_{x \rightarrow x_0} \frac{\|f(x) - A(x)\|}{\|x - x_0\|} &= 0 & A(x) &= L(x) + (f(x_0) - L(x_0)) = L(x - x_0) + f(x_0) \\ & & \lim_{x \rightarrow x_0} \frac{\|f(x) - (L(x - x_0) + f(x_0))\|}{\|x - x_0\|} &= 0 \end{aligned}$$



Differentiability

- Differentiable
 - A function f is said to be **differentiable** at x_0 if there is an affine function L that approximates f near x_0 ; that is, there exists $L: \mathbb{R}^n \rightarrow \mathbb{R}^m$ such that
- $$\lim_{x \rightarrow x_0} \frac{\|f(x) - (L(x - x_0) + f(x_0))\|}{\|x - x_0\|} = 0$$
- The linear transformation above is called the **derivative** of f at x_0 .
 - Any linear transformation can be represented by an **$m \times n$ matrix**.

$$Df(x_0) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x_0) & \dots & \frac{\partial f}{\partial x_n}(x_0) \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x_0) & \frac{\partial f_1}{\partial x_2}(x_0) & \dots & \frac{\partial f_1}{\partial x_n}(x_0) \\ \frac{\partial f_2}{\partial x_1}(x_0) & \frac{\partial f_2}{\partial x_2}(x_0) & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(x_0) & \frac{\partial f_m}{\partial x_2}(x_0) & \dots & \frac{\partial f_m}{\partial x_n}(x_0) \end{bmatrix}$$



Partial Derivative

- Derivative of $f: R^n \rightarrow R^m$ at x_0

$$Df(x_0) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x_0) & \cdots & \frac{\partial f}{\partial x_n}(x_0) \end{bmatrix}$$

- Partial derivative of $f: R^n \rightarrow R^m$ along e_j $\frac{\partial f}{\partial x_j}(x_0) = L e_j$

$x_j = x_0 + t e_j$, where $e_j = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$,
 $\Rightarrow \lim_{t \rightarrow 0} \frac{\|f(x_j) - (L e_j + f(x_0))\|}{t} = 0$ if $f(x) = \begin{bmatrix} f_1 \\ \vdots \\ f_m \end{bmatrix}$, then $\frac{\partial f}{\partial x_j}(x_0) = \begin{bmatrix} \frac{\partial f_1}{\partial x_j}(x_0) \\ \vdots \\ \frac{\partial f_m}{\partial x_j}(x_0) \end{bmatrix}$,
 $\Rightarrow \lim_{t \rightarrow 0} \frac{\|f(x_j) - f(x_0)\|}{t} = L e_j$. and Df is the Jacobian matrix.



Special Cases

- Special cases
 - For $f: R \rightarrow R$, $Df(x) = a$.
 - For $f: R^n \rightarrow R$, Df is a $1 \times n$ vector.
 - For $f: R^n \rightarrow R^m$, Df is a $m \times n$ matrix.

$$Df(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x) & \cdots & \frac{\partial f}{\partial x_n}(x) \end{bmatrix}$$

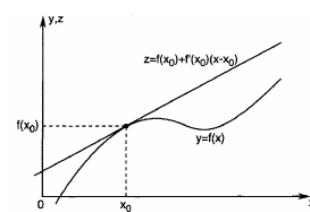


Figure 5.1 Illustration of the notion of the derivative



Gradient & Hessian Matrix

- Gradient

- If $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is differentiable at every point of its domain, then the gradient ∇f is defined by

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix} = Df(x)^T \quad \nabla f: \mathbb{R}^n \rightarrow \mathbb{R}^n$$

- Hessian Matrix

- If ∇f is differentiable,
- then f is twice differentiable.

$$\nabla^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$



Level Sets and Gradients

- Level Set

- The level set of a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ at level c is the set of points $S = \{x \mid f(x) = c\}$.

- Theorem

- The gradient vector ∇f is orthogonal or normal to an arbitrary smooth curve passing through x_0 on the level set S determined by $f(x) = f(x_0)$.

i.e. $\nabla f(x_0)^T (x - x_0) = 0$, if $\nabla f(x_0) \neq 0$.

Theorem

- Orthogonality of the gradient to the level set
- Gradient is the direction of **maximum rate** of increase of f at x_0 .

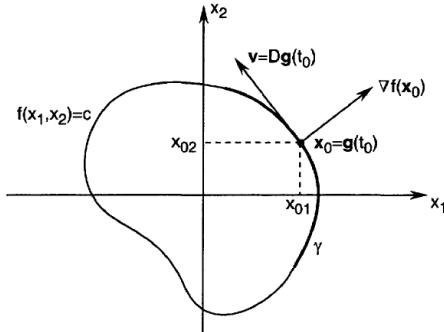


Figure 5.4 Orthogonality of the gradient to the level set

The graph of $f: \mathbb{R}^n \rightarrow \mathbb{R}$

- The graph of $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is the set $\{[x^T, f(x)]^T: x \in \mathbb{R}^n\} \subset \mathbb{R}^{n+1}$

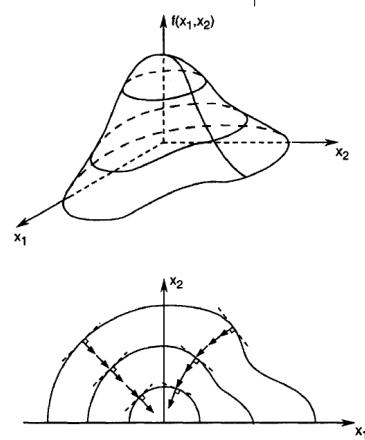


Figure 5.5 Illustration of a path of steepest ascent



Taylor's Series

- Theorem

$$f(x) = f(x_0) + \frac{(x-x_0)}{1!} f^{(1)}(x_0) + \frac{(x-x_0)^2}{2!} f^{(2)}(x_0) + \dots + \frac{(x-x_0)^{m-1}}{(m-1)!} f^{(m-1)}(x_0) + R_m,$$

where $f^{(i)}$ is the i th derivative of f , and

$$R_m = \frac{(x-x_0)^m}{m!} f^{(m)}(x_0 + \theta(x-x_0)),$$

with $\theta \in (0,1)$.