Introduction to Machine Learning - CS725
Instructor: Prof. Ganesh Ramakrishnan
Lecture 9 - Optimization Foundations Applied to Regression Formulations

Building on questions on Least Squares Linear Regression

1. Is there a probabilistic interpretation?
   - Gaussian Error, Maximum Likelihood Estimate
2. Addressing overfitting
   - Bayesian and Maximum Aposteriori Estimates, Regularization, Support Vector Regression
3. How to minimize the resultant and more complex error functions?
   - Level Curves and Surfaces, Gradient Vector, Directional Derivative, Gradient Descent Algorithm, Convexity, Necessary and Sufficient Conditions for Optimality

KKT Conditions

① Dual of SVR .. Kernels

② Equivalence of penalized & constrained regression

SVR objective

- 1-norm Error, and L_2 regularized:
  - $\min_{\mathbf{w},b,\xi_i,\xi_i^*} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i + \xi_i^*)$
    s.t. $\forall i$,
    $y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b \leq \epsilon + \xi_i$,
    $b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i \leq \epsilon + \xi_i^*$,
    $\xi_i, \xi_i^* \geq 0$

    } Number of constraints = 2 · # of examples (m)
- 2-norm Error, and L_2 regularized:
  - $\min_{\mathbf{w},b,\xi_i,\xi_i^*} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i^2 + \xi_i^{*2})$
    s.t. $\forall i$,
    $y_i - \mathbf{w}^\top\phi(x_i) - b \leq \epsilon + \xi_i$,
    $b + \mathbf{w}^\top\phi(x_i) - y_i \leq \epsilon + \xi_i^*$
  - Here, the constraints $\xi_i, \xi_i^* \geq 0$ are not necessary

Need for Optimization so far

- **Unconstrained (Penalized) Optimization:**

$$\mathbf{w}_{Reg} = \arg\min_{\mathbf{w}} \; ||\Phi\mathbf{w} - \mathbf{y}||_2^2 + \Omega(\mathbf{w})$$

- **Constrained Optimization 1:**

$$\mathbf{w}_{Reg} = \arg\min_{\mathbf{w}} \; ||\Phi\mathbf{w} - \mathbf{y}||_2^2$$

$$\textit{such that } \Omega(\mathbf{w}) \leq \theta$$

- **Constrained Optimization 2 ($t = 1$ or 2):**

$$\arg\min_{\mathbf{w}, b, \xi_i, \xi_i^*} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i (\xi_i^t + \xi_i^{*t})$$

s.t. $\forall i,\ y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon + \xi_i;\ b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i \leq \epsilon + \xi_i^*$

- **Equivalence**: λ (Penalized) $\equiv$ θ (Constrained)
- **Duality**: Dual of Support Vector Regression

Solving Unconstrained Minimization Problem

- Intuitively: Minimize by setting derivative (gradient) to 0 and hoping to find **closed form** solution.
- When is such a solution a global minimum?
- For most optimization problems, finding closed form solutions is difficult. Even for linear regression (for which closed form solution exists), are there alternative methods? w^* s.t $\nabla f = 0$
  - Eg: Consider, $\mathbf{y} = \phi \mathbf{w}$,where ϕ is a matrix with full column rank, the least squares solution, $\mathbf{w}^* = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y}$. Now, imagine that ϕ is a very large matrix. with say, 100,000 columns and 1,000,000 rows. Computation of closed form solution might be challenging.
- How about iterative methods?

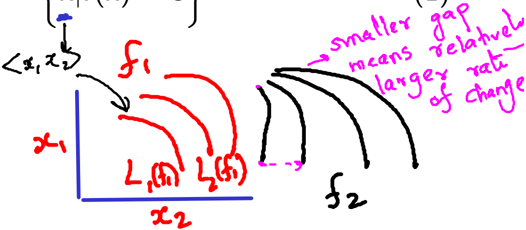
$$w^{new} = w^{old} + \Delta w$$

Foundations: Level curves and surfaces

- A level curve of a function $\mathbf{f}(\mathbf{x})$ is defined as a curve along which the value of the function remains unchanged while we change the value of its argument x.
- Formally we can define a level curve as :

$$L_c(\mathbf{f}) = \left\{ \mathbf{x} | \mathbf{f}(\mathbf{x}) = \mathbf{c} \right\} \tag{1}$$

where c is a constant.



Foundations: Level curves and surfaces

- Example of different level curves for a single function

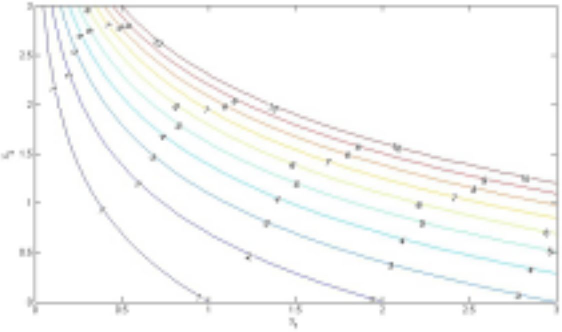


Figure 1: 10 level curves for the function $\mathbf{f}(\mathbf{x_1}, \mathbf{x_2}) = \mathbf{x_1} \mathbf{e}^{\mathbf{x_2}}$ (Figure 4.12 from `https://www.cse.iitb.ac.in/~CS725/notes/classNotes/BasicsOfConvexOptimization.pdf`)

Foundations: Directional Derivatives

- Directional derivative: Rate at which the function changes at a given point $\mathbf{x}$ in a given direction $\mathbf{v}$
- The *directional derivative* of a function f in the direction of a unit vector $\mathbf{v}$ at a point $\mathbf{x}$ can be defined as :

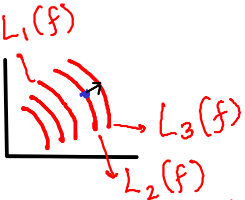
$$D_{\mathbf{v}}(f, \mathbf{x}) = \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{v}) - \mathbf{f}(\mathbf{x})}{h} \tag{2}$$

$$s.t. \ ||\mathbf{v}||_2 = \mathbf{1} \tag{3}$$

Foundations: Gradient Vector

claim: $D_v(f, x) = v^T \nabla f(x)$

- The **g**radient vector of a function f at a point $\mathbf{x}$ is defined as:



$$\nabla f_{\mathbf{x}^*} = \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ . \\ . \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{bmatrix} \epsilon \mathbb{R}^n \tag{4}$$

$\|\nabla f_x\|_2$

- Magnitude (euclidean norm) of gradient vector at any point indicates maximum value of directional derivative at that point
- Direction of gradient vector indicates direction of this maximal directional derivative at that point. $\Big\} \rightarrow \frac{\nabla f_x}{\|\nabla f_x\|}$

- The figure below illustrates the gradient vector for the same level curves

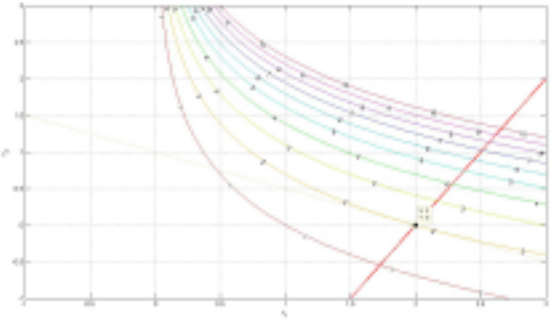
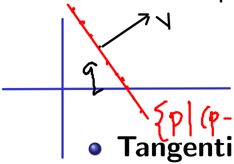


Figure 2: The level curves along with the gradient vector at (2, 0). Note that the gradient vector is perpendicular to the level curve $x_1 e^{x_2} = 2$ at (2, 0)

Hyperplanes

- A hyperplane in an n-dimensional Euclidean space is a flat, n-1 dimensional subset of that space that divides the space into two disjoint half-spaces.
- Technically, a hyperplane is a set of points whose direction *w.r.t.* a point $\mathbf{q}$ is orthogonal to a vector $\mathbf{v}$:

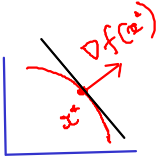


$\{p \mid (p-q)^T v = 0\}$

$$H_{\mathbf{v},\mathbf{q}} = \left\{ \mathbf{p} \,\middle|\, (\mathbf{p}-\mathbf{q})^{\mathbf{T}}\mathbf{v} = \mathbf{0} \right\} \tag{5}$$

such that $\quad p, q, v \in \mathbb{R}^n$

- **Tangential Hyperplane:** Plane orthogonal to the gradient vector at $\mathbf{x}^*$.



$$TH_{x^*} = H_{\nabla f(x^*), x^*} = \{p \mid (p - x^*)^T \nabla f(x^*) = 0\}$$

Hyperplanes

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- Technically, a hyperplane is a set of points whose direction *w.r.t.* a point **q** is orthogonal to a vector **v**:

$$H_{\mathbf{v},\mathbf{q}} = \left\{ \mathbf{p} \mid (\mathbf{p} - \mathbf{q})^{\mathbf{T}} \mathbf{v} = \mathbf{0} \right\} \tag{5}$$

- **Tangential Hyperplane:** Plane orthogonal to the gradient vector at $\mathbf{x}^*$.

$$TH_{\mathbf{x}^*} = \left\{ \mathbf{p} \mid (\mathbf{p} - \mathbf{x}^*)^{\mathbf{T}} \nabla \mathbf{f}(\mathbf{x}^*) = \mathbf{0} \right\} \tag{6}$$

We recall that the problem was to find **w** such that (L2 regularized linear regression)

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \|\Phi\mathbf{w} - \mathbf{y}\|^2 + \lambda||\mathbf{w}||^2 \quad (7)$$

$$= \arg\min_{\mathbf{w}} (\mathbf{w}^T\Phi^T\Phi\mathbf{w} - 2\mathbf{w}^T\phi\mathbf{y} + \mathbf{y}^T\mathbf{y} + \lambda||\mathbf{w}||^2) \quad (8)$$

Foundations: Gradient Vector

- Magnitude (euclidean norm) of gradient vector at any point indicates maximum value of directional derivative at that point
- Thus, at the point of minimum of a differentiable minimization objective (such as least squares for regression), ...

We expect $\nabla f(w^*) = 0$

- *If* $\nabla f(\mathbf{w}^*)$ *is defined &* $\mathbf{w}^*$ *is local minimum/maximum, then* $\nabla f(\mathbf{w}^*) = 0$ (A necessary condition) (Cite : Theorem 60) of `CS725/notes/classNotes/BasicsOfConvexOptimization.pdf`
- Given that

Quadratic in ω .. $\frac{d\,\phi^2\omega^2}{d\omega} = 2\phi^2\omega$

$$f(\mathbf{w}) = \arg\min_{\mathbf{w}}(\mathbf{w}^T\Phi^T\Phi\mathbf{w} - 2\mathbf{w}^T\Phi^T\mathbf{y} - \mathbf{y}^T\mathbf{y} + \lambda||\mathbf{w}||^2$$

$\implies$ ....

$$\nabla f(\omega) = \begin{bmatrix} \partial f_{\omega_1} \\ \partial f_{\omega_2} \\ \vdots \\ \partial f_{\omega_n} \end{bmatrix} = \nabla_\omega(\omega^T\phi^T\phi\omega) - \nabla_\omega(2\omega^T\phi y) + \nabla_\omega(\lambda\omega^T\omega)$$

$$= 2\phi^T\phi\omega - 2\phi^T y + 2\lambda\omega$$

- We would have

....

$\implies$ ....

$\implies$ ....

Foundations: Necessary condition 1

- *If* $\nabla f(\mathbf{w}^*)$ *is defined &* $\mathbf{w}^*$ *is local minimum/maximum, then* $\nabla f(\mathbf{w}^*) = 0$ (A necessary condition) (Cite : Theorem 60) CS725/notes/classNotes/BasicsOfConvexOptimization.pdf
- Given that

$$f(\mathbf{w}) = \arg\min_{\mathbf{w}} (\mathbf{w}^T\Phi^T\Phi\mathbf{w} - 2\mathbf{w}^T\Phi^T\mathbf{y} - \mathbf{y}^T\mathbf{y} + \lambda||\mathbf{w}||^2) \quad (9)$$

$$\implies \underbrace{\nabla f(\mathbf{w}) = 2\Phi^T}_{\text{Disappears at } w^*}\Phi\mathbf{w} - 2\Phi^T\mathbf{y} + 2\lambda\mathbf{w} \quad (10)$$

- We would have

$$\nabla f(\mathbf{w}^*) = 0 \quad (11)$$

$$\implies \underline{2(\Phi^T}\Phi + \lambda I)\mathbf{w}^* - 2\Phi^T\mathbf{y} = 0 \quad (12)$$

$$\implies \mathbf{w}^* = \underbrace{(\Phi^T\Phi + \lambda I)^{-1}}_{\text{Assuming invertibility}}\Phi^T\mathbf{y} \quad (13)$$

$2\lambda w = 2\lambda I w$ .. Different representation

Foundations: Necessary Condition 2

Necessary for Local min that $\nabla^2 f(x^*) \succeq 0$

- *Is* $\nabla^2 f(\mathbf{w}^*)$ *positive definite ?*
  i.e. $\forall \mathbf{x} \neq 0$, *is* $\mathbf{x}^T \nabla f(\mathbf{w}^*)\mathbf{x} > 0$? (A sufficient condition for local minimum)
  (Note : Any positive definite matrix is also positive semi-definite)
  (`Cite : Section 3.12 & 3.12.1`)[1]

$$\nabla^2 f(\omega) = \begin{bmatrix} \frac{\partial^2 f(\omega)}{\partial \omega_i^2} & \cdots \\ & \frac{\partial^2 f(\omega)}{\partial \omega_i \omega_j} \end{bmatrix} \Longrightarrow$$

Hessian is symmetric

$\nabla f(\omega) = 2(\phi^T\phi + \lambda I)\omega - 2\underbrace{\phi^T y}$

$\nabla^2 f(\omega) = 2(\phi^T\phi + \lambda I)$

can be ignored for $\nabla^2 f(\omega)$

$\forall v \neq 0 \quad v^T \nabla^2 f(\omega) v \geq 0$

Because $2\|\phi v\|_2^2 + \lambda \|v\|_2^2 \geq 0$

- And if Φ **has full column rank** ,

. . . .

$\therefore$ If $\mathbf{x} \neq 0$, $\mathbf{x}^T \nabla^2 f(\mathbf{w}^*)\mathbf{x} > 0$

[1] `CS725/notes/classNotes/LinearAlgebra.pdf`

Foundations: Necessary Condition 2

- *Is* $\nabla^2 f(\mathbf{w}^*)$ *positive definite ?*
  i.e. $\forall \mathbf{x} \neq 0$, *is* $\mathbf{x}^T \nabla f(\mathbf{w}^*)\mathbf{x} > 0$? (A sufficient condition for local minimum)
  (Any positive definite matrix is also positive semi-definite)
  `(Cite : Section 3.12 & 3.12.1)`[2]

$$\nabla^2 f(\mathbf{w}^*) = 2\Phi^T\Phi + 2\lambda I \quad (14)$$

$$\implies \mathbf{x}^T\nabla^2 f(\mathbf{w}^*)\mathbf{x} = 2\mathbf{x}^T(\Phi^T\Phi + \lambda I)\mathbf{x} \quad (15)$$

$$= 2\left((\Phi + \sqrt{\lambda} I)\mathbf{x}\right)^T \Phi\mathbf{x} \quad (16)$$

$$= 2\left\|(\Phi + \sqrt{\lambda} I)\mathbf{x}\right\|^2 \geq 0 \quad (17)$$

(About positive semidefiniteness)

- And with $\lambda = 0$, if Φ **has full column rank** ,

$\|p\| = 0$ iff $p = 0$
ie $(\Phi + \sqrt{\lambda} I)x = 0$
$\Leftrightarrow x^T \nabla^2 f(w^*) x = 0$

$$\Phi\mathbf{x} = 0 \quad \textit{iff} \quad \mathbf{x} = 0 \quad (18)$$

$\Rightarrow$
$x^T \nabla^2 f(w^*) x = 0$ iff $x = 0$
$\Rightarrow \nabla^2 f(w^*) \succ 0$

$\therefore$ If $\mathbf{x} \neq 0$, $\mathbf{x}^T\nabla^2 f(\mathbf{w}^*)\mathbf{x} > 0$

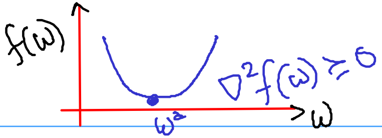
[2] `CS725/notes/classNotes/LinearAlgebra.pdf`

① with any $\lambda \geq 0$ $\nabla^2 f(w) \succeq 0$ $\forall\, w \in \mathbb{R}^n$

$\Downarrow$

The ridge regression objective function is convex everywhere (& $\therefore$ also convex at w^*)

global min



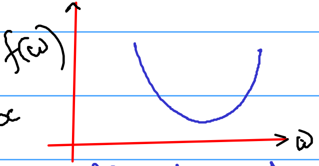
Necessary condition for local min at w^* is "convex" or cup-shaped curvature at w^*

② with $\lambda = 0$ ∧ & Φ full col. rank $\nabla^2 f(w) \succ 0$

$\Downarrow$

The ridge regression objective function is strictly convex everywhere (& $\therefore$ also at w^*)

global min



Sufficient condition for local (& even global) min at w^* is strictly convex curvature

New takeaways:

1. $\nabla^2 f(w) \succeq 0 \quad \forall w \Rightarrow f$ is convex everywhere & $\therefore$ necessary condition for local min to become global min

2. $\nabla^2 f(w) \succ 0 \quad \forall w \Rightarrow f$ is strictly convex everywhere & sufficient condition for local min to become global min

3. If $\lambda > 0$, $\nabla^2 f(w)$ tends to become "more" positive definite

Example of linearly correlated features

- Example where Φ doesn't have a full column rank,

$$\Phi = \begin{bmatrix} x_1 & x_1^2 & x_1^2 & x_1^3 \\ x_2 & x_2^2 & x_2^2 & x_2^3 \\ \vdots & \vdots & \vdots & \vdots \\ x_n & x_n^2 & x_n^2 & x_n^3 \end{bmatrix} \tag{19}$$

- This is the simplest form of linear correlation of features, and it is not at all desirable.
- Effect of a nonzero λ with such Φ is that

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- This is the simplest form of linear correlation of features, and it is not at all desirable.
- Effect of a nonzero λ with such Φ is that it tends to make the Hessian more positive definite

Do Closed-form solutions Always Exist?

- Linear regression and Ridge regression both have closed-form solutions
  - For linear regression,

$$w^* = (\Phi^\top \Phi)^{-1} \Phi^\top y$$

  - For ridge regression,

$$w^* = (\Phi^\top \Phi + \lambda I)^{-1} \Phi^\top \mathbf{y}$$

  (for linear regression, $\lambda = 0$)

- What about optimizing the formulations (constrained/penalized) of Lasso (L_1 norm)? And support-based penalty (L_0 norm)?: Also requires tools of Optimization/duality