UCLA Samueli Computer Science

CS M146 Discussion: Week 3

Perceptron, Linear Models, Optimization

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Friday, 01/22/2021

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Roadmap

- Announcement
- Perceptron & Linear Models
- Optimization, MLE

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Announcements

- 5:00 pm PST, Jan. 22: Weekly Quiz 3 released on Gradescope.
- **11:59 pm PST, Jan. 24 (Sunday):** Weekly quiz 3 closed on Gradescope!
  - Start the quiz before **11:00 pm PST, Jan. 24** to have the full 60-minute time
- Problem set 1 released on campuswire/CCLE, submission on Gradescope.
  - Please assign pages of your submission with corresponding problem set outline items on GradeScope.
  - You do not need to submit code, only the results required by the problem set
  - Due on **11:59pm PST, Jan. 29 (Friday)**

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About Quiz 3

- Quiz release date and time: **Jan 22, 2021 (Friday) 05:00 PM PST**
- Quiz due/close date and time: **Jan 24, 2021 (Sunday) 11:59 PM PST**
- You will have up to **60 minutes** to take this exam. → Start before **11:00 PM** Sunday
- You can find the exam entry named "Week 3 Quiz" on GradeScope.
- Topics: **Perceptron, Linear Models**
- Question Types
  - True/false, multiple choices, and auto-graded short answers (fill blanks)
  - Some questions may include several subquestions.
- Some light calculations are expected. Some scratch paper and one scientific calculator (physical or online) are recommended for preparation.

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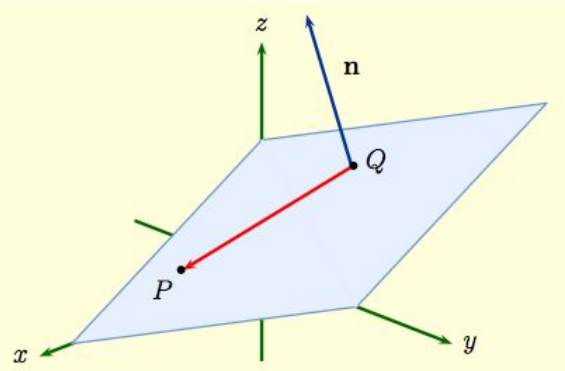
*One more quiz of K-NN

- True/False: The training error of K-NN will be zero when K = 1, irrespective of the dataset.

Math Reminder: Normal vector and plane

- A normal vector is a vector perpendicular to another object, such as a surface or plane.



Let $Q(a,\ b,\ c)$ be a fixed point in the plane, $P(x,\ y,\ z)$ an arbitrary point in the plane, and $\mathbf{n} = \langle A,\ B,\ C \rangle$ the normal to the plane. If

$$\mathbf{b} = \langle a,\ b,\ c \rangle, \qquad \mathbf{r} = \langle x,\ y,\ z \rangle,$$

the vector

$$\overrightarrow{QP} = \mathbf{r} - \mathbf{b} = \langle x - a,\ y - b,\ z - c \rangle$$

lies in the plane, and is **perpendicular** to $\mathbf{n}$.

Thus $\mathbf{n} \cdot (\mathbf{r} - \mathbf{b}) = 0$. In terms of coordinates, this becomes

$$\langle A,\ B,\ C \rangle \cdot \langle x - a,\ y - b,\ z - c \rangle = 0,$$

where $\mathbf{n} = \langle A,\ B,\ C \rangle$. In other words, we get the **point-normal** equation

$$A(x - a) + B(y - b) + C(z - c) = 0.$$

for a plane.

Credit: https://web.ma.utexas.edu/users/m408m/Display12-5-4.shtml

Math Reminder: Normal vector and plane

- A normal vector is a vector perpendicular to another object, such as a surface or plane.

As promised, we return the the question of finding the equation for a plane from the location of three points, say

$$Q(x_1,\, y_1,\, z_1)\,, \qquad R(x_2,\, y_2,\, z_2)\,, \qquad S(x_3,\, y_3,\, z_3)$$

The fact that the cross-product $\mathbf{a} \times \mathbf{b}$ is perpendicular to both $\mathbf{a}$ and $\mathbf{b}$ makes it very useful when dealing with normals to planes.

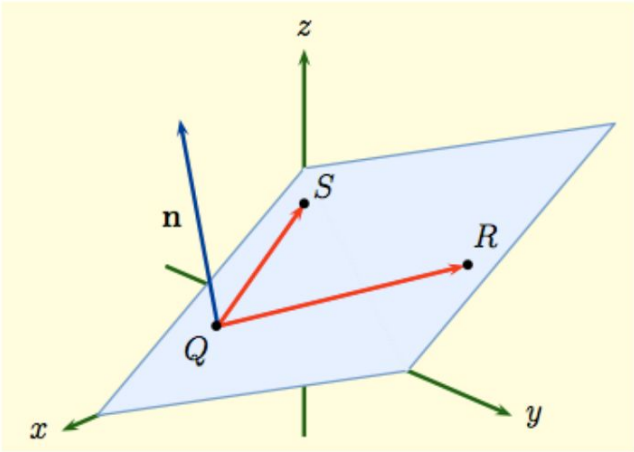
Let

$$\mathbf{b} = \langle\, x_1,\, y_1,\, z_1 \,\rangle\,, \quad \mathbf{r} = \langle\, x_2,\, y_2,\, z_2 \,\rangle\,, \quad \mathbf{s} = \langle\, x_3,\, y_3,\, z_3 \,\rangle.$$

The vectors

$$\overrightarrow{QR} \;=\; \mathbf{r} - \mathbf{b}\,, \qquad \overrightarrow{QS} \;=\; \mathbf{s} - \mathbf{b}\,,$$

then lie in the plane. The normal to the plane is given by the cross product $\mathbf{n} = (\mathbf{r} - \mathbf{b}) \times (\mathbf{s} - \mathbf{b})$. Once this normal has been calculated, we can then use the point-normal form to get the equation of the plane passing through Q, R, and S.



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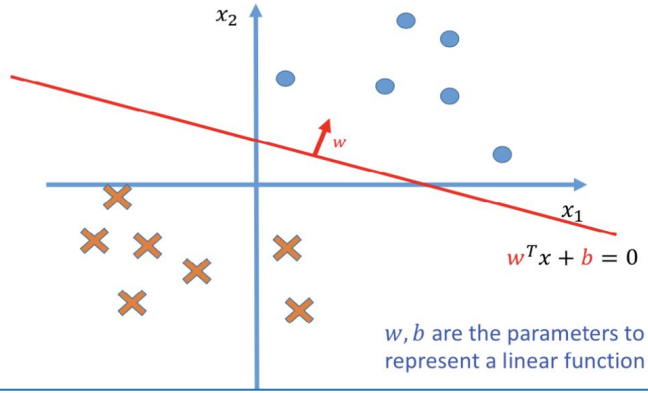
Math Reminder: Normal vector and plane

- Demo Calculation Example

Perceptron: Overview

- Instance (feature vectors): $\boldsymbol{x} \in \mathbb{R}^{\mathrm{D}}$
- Label: $y \in \{-1, +1\}$
- Model/Hypotheses:
  $H = \{h | h : \mathbb{X} \to \{-1, +1\}, h(\boldsymbol{x}) = sign(\sum_{d=1}^{D} w_d x_d + b)\}$.
- Learning goal: $y = h(\boldsymbol{x})$
  - Learn $w_1, \ldots, w_D, b$.
  - Parameters: $w_1, \ldots, w_D, b$.
  - $\boldsymbol{w}$: weights, b: bias



Iteratively solving one case at a time

- REPEAT
- Pick a data point $\boldsymbol{x}_n$
- Compute $a = \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n$ using the *current* $\boldsymbol{w}$
- If $ay_n > 0$, do nothing. Else,

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + y_n \boldsymbol{x}_n$$

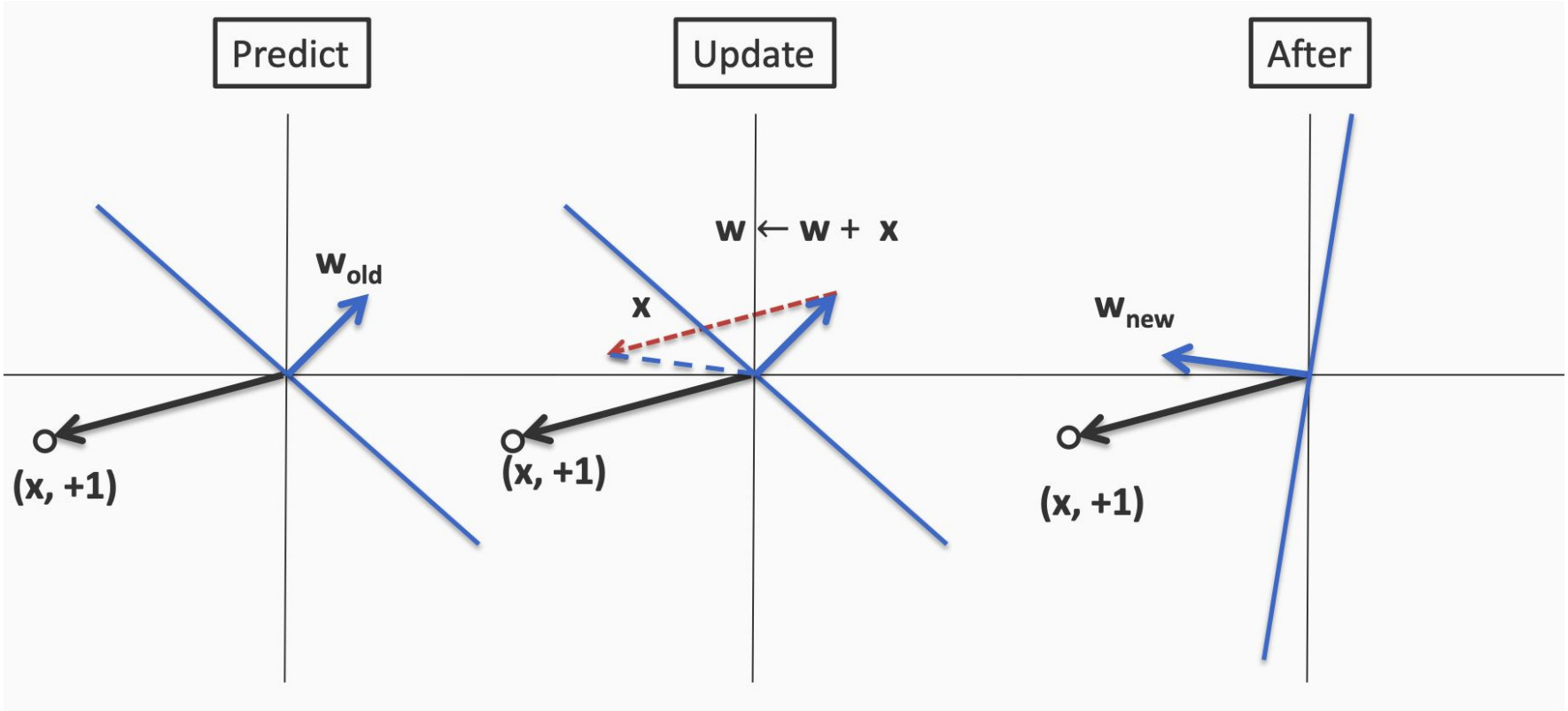
- UNTIL converged.

Perceptron: Convergence

- If training data is **not linearly separable**, the algorithm does not converge.
- If the training data is **linearly separable**, the algorithm stops in a finite number of steps (converges).

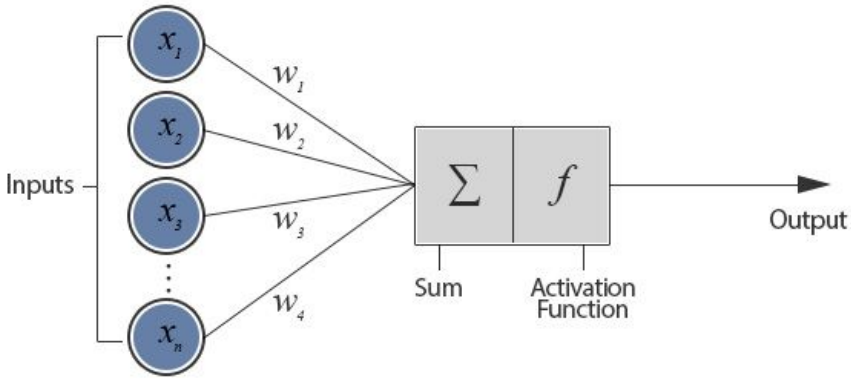
- Let $\{(\boldsymbol{x}_1, y_1), \cdots, (\boldsymbol{x}_\mathsf{N}, y_\mathsf{N})\}$ be a sequence of training examples such that $\|\boldsymbol{x}_n\|_2 \leq R$ and label $y_n \in \{-1, +1\}$.
- Suppose there exists a unit vector $\boldsymbol{u} \in \mathbb{R}^D$ such that for some $\gamma > 0$, we have $y_n \boldsymbol{u}^\mathrm{T} \boldsymbol{x}_n \geq \gamma$.
- Then the Perceptron algorithm will make at most $\frac{R^2}{\gamma^2}$ mistakes on the training sequence.

Perceptron: Update (Geometry)

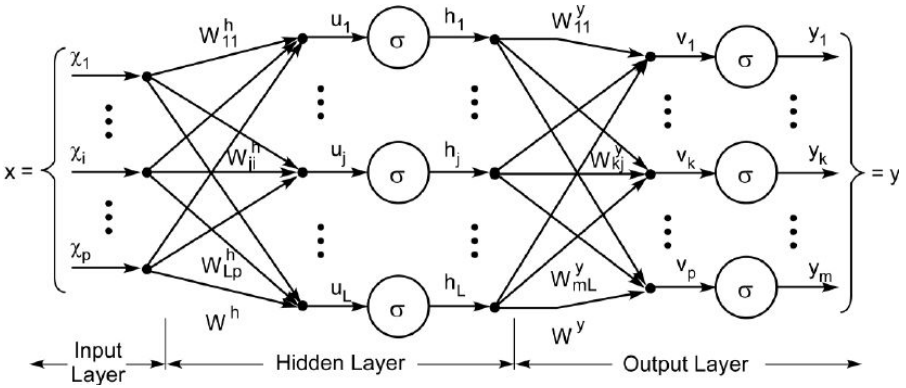


Perceptron: Connect to Neural Network

A Single Perceptron



Multi-layer Neural Network



Question: Can a single perceptron classify XOR data? How about 2-layer perceptrons?

Logistic Regression: Overview

Probability of a single training sample $(\boldsymbol{x}_n, y_n)$

$$p(y_n|\boldsymbol{x}_n; b, \boldsymbol{w}) = \begin{cases} h_{\boldsymbol{w},b}(\boldsymbol{x}_n) = \sigma(b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n) & \text{if} \quad y_n = 1 \\ = 1 - h_{\boldsymbol{w},b}(\boldsymbol{x}_n) = 1 - \sigma(b + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n) & \text{otherwise} \end{cases}$$

Compact expression, exploring that y_n is either 1 or 0

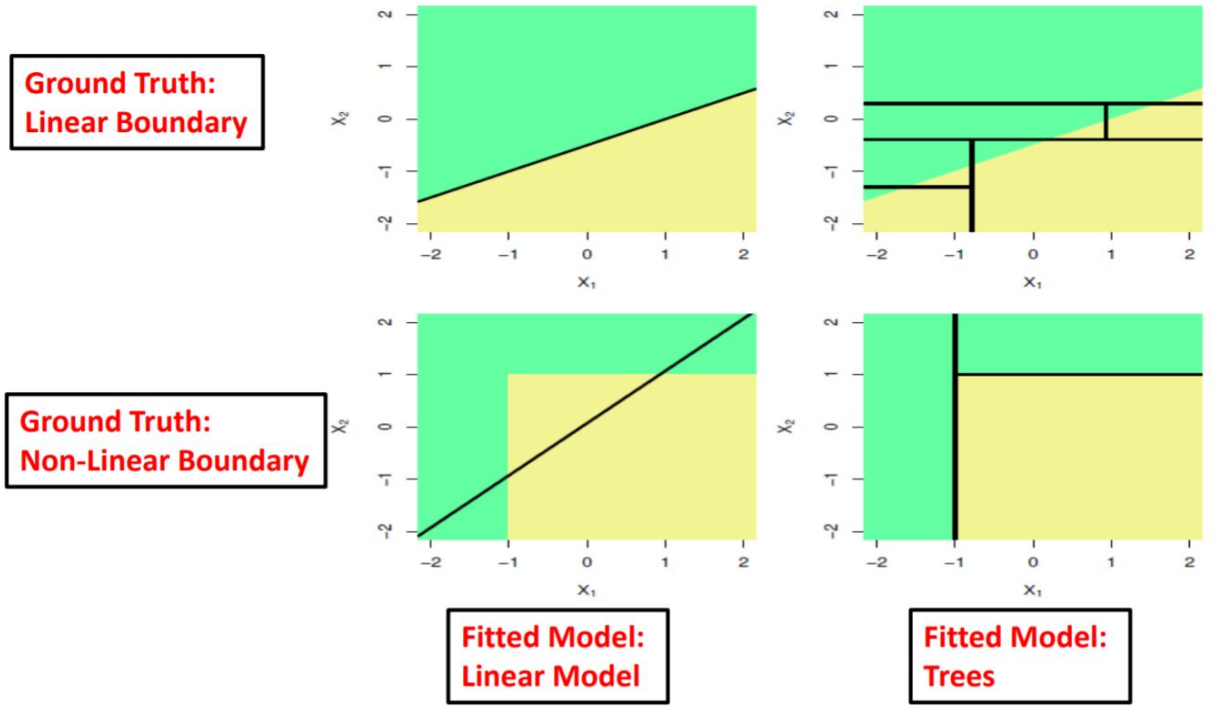
$$p(y_n|\boldsymbol{x}_n; b; \boldsymbol{w}) = h_{\boldsymbol{w},b}(\boldsymbol{x}_n)^{y_n}[1 - h_{\boldsymbol{w},b}(\boldsymbol{x}_n)]^{1-y_n}$$

Log-likelihood of the whole training data $\mathcal{D}$

$$l(\boldsymbol{w}, b) = \sum_n \{y_n \log h_{\boldsymbol{w},\boldsymbol{b}}(\boldsymbol{x}_n) + (1 - y_n) \log[1 - h_{\boldsymbol{w},b}(\boldsymbol{x}_n)]\}$$

Linear Models

- Compare: Decision Tree, Nearest Neighbors, Perceptron



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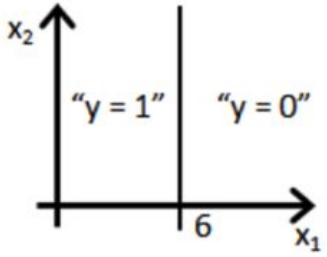
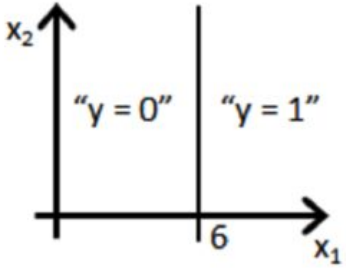
Decision Boundary: Quiz

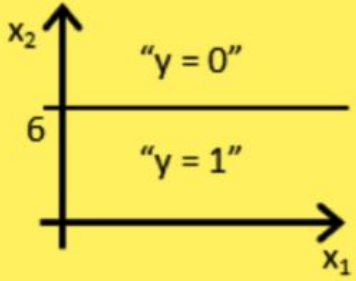
Suppose you train a logistic classifier $h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$. Suppose $\theta_0 = 6, \theta_1 = 0, \theta_2 = -1$. Which of the following figures represents the decision boundary found by your classifier?

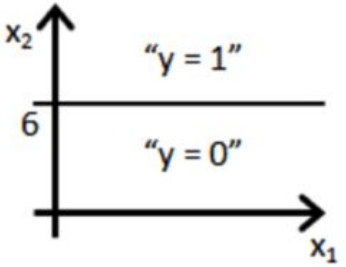
Decision Boundary: Quiz

Suppose you train a logistic classifier $h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$. Suppose $\theta_0 = 6, \theta_1 = 0, \theta_2 = -1$. Which of the following figures represents the decision boundary found by your classifier?









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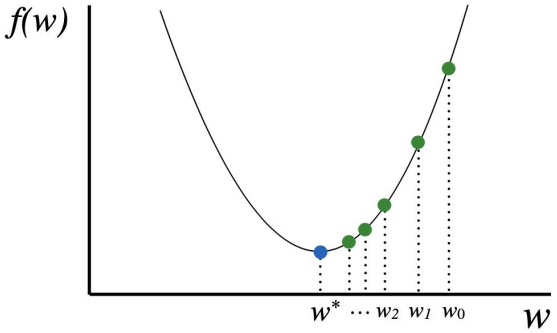
Unconstrained Optimization

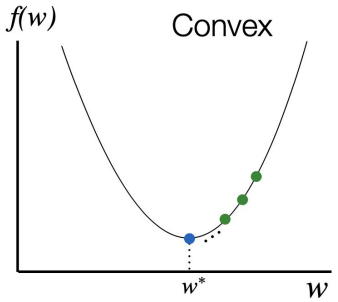
- Convex Function and Convexity
- Closed-form solution
- Gradient Descent
- Newton’s methods

Gradient Descent

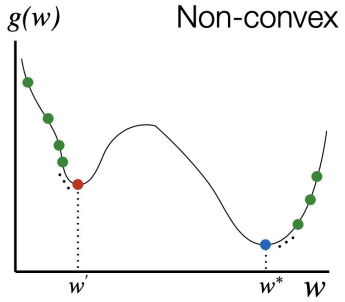
Start at a random point
Repeat
    Determine a descent direction
    Choose a step size
    Update
Until stopping criterion is satisfied



Where Will We Converge?



Any local minimum is a global minimum



Multiple local minima may exist

Newton's Method (Optional)

Definition:

$$\beta^{\text{new}} = \beta^{\text{old}} - \left(\frac{\partial^2 L(\beta)}{\partial\beta\partial\beta^T}\right)^{-1} \frac{\partial L(\beta)}{\partial\beta}$$

Apply Newton's methods on single variable to find minima:

$$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$$

From single variable to Multivariate Newton-Raphson Method

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Newton's Method: Steps (Optional)

1. Initialize $x^{(0)}$
2. Calculate $\nabla f(x)$
3. Calculate $F(x)$
4. Initialize step$n = 0$ and start loops
   a. Calculate $\nabla f(x^{(n)})$
   b. Calculate $F(x^{(n)})$
   c. Calculate $[F(x^{(n)})]^{-1}$
   d. Update: $x^{(n+1)} = x^{(n)} - [F(x^{(n)})]^{-1} \cdot \nabla f(x^{(n)})$
   e. Update: $n = n + 1$
5. Exit Loop

Newton's Method: Example (Optional)

$$x^{(0)} = [3, -1, 0]$$

$$f(x_1, x_2, x_3) = (x_1 + 10x_2)^2 + 5(x_1 - x_3)^2 + (x_2 - 2x_3)^4$$

Newton's Method Example in one step:

- ➔ Calculate $\nabla f(x^{(n)})$
- ➔ Calculate $F(x^{(n)})$
- ➔ Calculate $[F(x^{(n)})]^{-1}$
- ➔ Update: $x^{(n+1)}$
- ➔ Update: $n = n + 1$

$$\nabla f(x^{(0)}) = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \frac{\partial f}{\partial x_3}\right] = [16, -144, 22]$$

$$F(x^{(0)}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_1 \partial x_3} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \frac{\partial^2 f}{\partial x_2 \partial x_3} \\ \frac{\partial^2 f}{\partial x_3 \partial x_1} & \frac{\partial^2 f}{\partial x_3 \partial x_2} & \frac{\partial^2 f}{\partial x_3^2} \end{bmatrix} = \begin{bmatrix} 12 & 20 & -10 \\ 20 & 22 & -24 \\ -10 & -24 & 48 \end{bmatrix}$$

$$[F(x^{(0)})]^{-1} = \begin{bmatrix} -0.079 & 0.119 & 0.043 \\ 0.119 & -0.079 & -0.015 \\ 0.043 & -0.015 & 0.023 \end{bmatrix}$$

$$x^{(1)} = x^{(0)} - [F(x^{(0)})]^{-1} \cdot \nabla f(x^{(0)})$$

$$n = 1$$

Maximum Likelihood Estimation

Definition: The maximum likelihood estimator (MLE) $\hat{\theta}$, is the value of θ that maximizes $L(\theta)$.

The log-likelihood function is defined by $l(\theta) = \log L(\theta)$. Its maximum occurs at the same place as that of the likelihood function.

- Using logs simplifies mathemetical expressions (converts exponents to products and products to sums)
- Using logs helps with numerical stabilitity

The same is true of the likelihood function times any constant. Thus we shall often drop constants in the likelihood function.

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MLE: Logistic Regression

- Model

$$y = \sigma(X) = \frac{1}{1 + e^{-X^T \beta}}$$

- Original Objective

$$J(\beta) = -\frac{1}{n} \sum_i \left(y_i x_i^T \beta - \log\left(1 + \exp\{x_i^T \beta\}\right)\right)$$

MLE: Logistic Regression

$$h_\theta(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}},$$

where

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

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

MLE: Logistic Regression

$$
\begin{aligned}
P(y = 1 \mid x; \theta) &= h_\theta(x) \\
P(y = 0 \mid x; \theta) &= 1 - h_\theta(x)
\end{aligned}
$$

$$p(y \mid x; \theta) = (h_\theta(x))^y \, (1 - h_\theta(x))^{1-y}$$

Assuming that the m training examples were generated independently, we can then write down the likelihood of the parameters as

$$
\begin{aligned}
L(\theta) &= p(\vec{y} \mid X; \theta) \\
&= \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta) \\
&= \prod_{i=1}^{m} \left(h_\theta(x^{(i)})\right)^{y^{(i)}} \left(1 - h_\theta(x^{(i)})\right)^{1-y^{(i)}}
\end{aligned}
$$

As before, it will be easier to maximize the log likelihood:

$$
\begin{aligned}
\ell(\theta) &= \log L(\theta) \\
&= \sum_{i=1}^{m} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)}))
\end{aligned}
$$

Constrained Optimization

- Lagrange Multiplier

$$\mathcal{L}(x, y, \lambda) = f(x, y) - \lambda g(x, y)$$

maximize $f(x, y)$
subject to: $g(x, y) = 0$

$$\nabla_{x,y,\lambda} \mathcal{L}(x, y, \lambda) = 0 \iff \begin{cases} \nabla_{x,y} f(x, y) = \lambda \nabla_{x,y} g(x, y) \\ g(x, y) = 0 \end{cases}$$

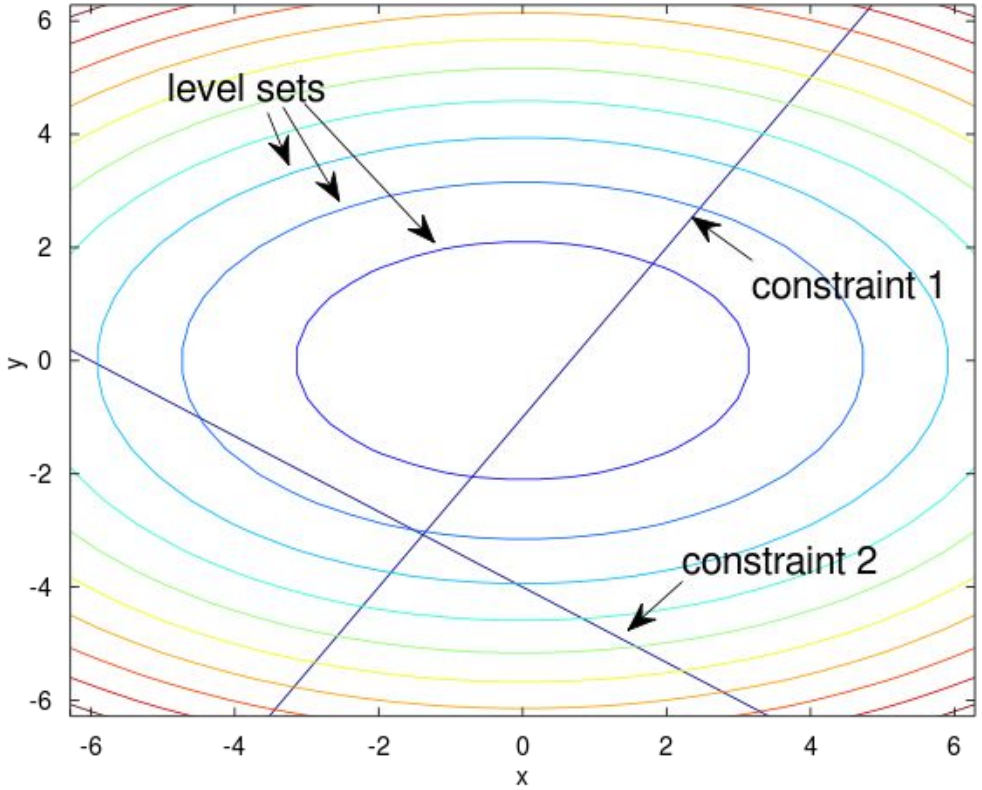
$$\nabla f(\mathbf{x}) = \sum_{k=1}^{M} \lambda_k \nabla g_k(\mathbf{x}) \iff \nabla f(\mathbf{x}) - \sum_{k=1}^{M} \lambda_k \nabla g_k(\mathbf{x}) = 0.$$

- Considering multiple constraints

$$\mathcal{L}\left(x_1, \ldots, x_n, \lambda_1, \ldots, \lambda_M\right) = f\left(x_1, \ldots, x_n\right) - \sum_{k=1}^{M} \lambda_k g_k\left(x_1, \ldots, x_n\right)$$

$$\nabla_{x_1,\ldots,x_n,\lambda_1,\ldots,\lambda_M} \mathcal{L}(x_1, \ldots, x_n, \lambda_1, \ldots, \lambda_M) = 0 \iff \begin{cases} \nabla f(\mathbf{x}) - \sum_{k=1}^{M} \lambda_k \nabla g_k(\mathbf{x}) = 0 \\ g_1(\mathbf{x}) = \cdots = g_M(\mathbf{x}) = 0 \end{cases}$$

Constrained Optimization

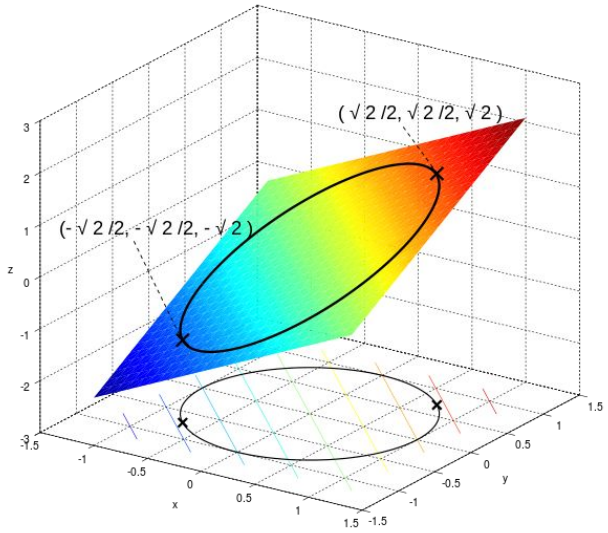


Lagrange Multiplier

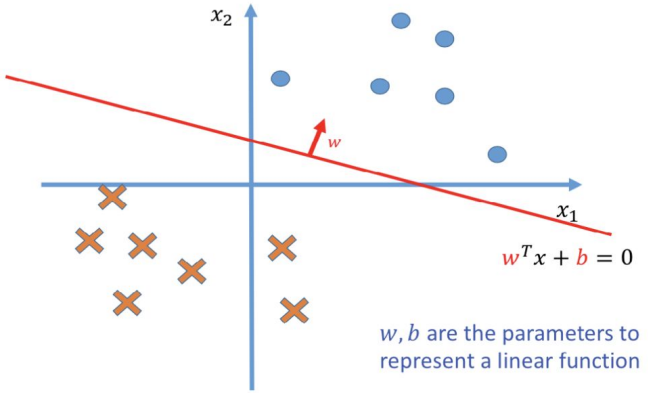
- Example:

$$f(x, y) = x + y$$

$$\text{Constraint} : g(x, y) = x^2 + y^2 = 1$$



Lagrange Multiplier: Connect to SVM *



Original optimization problem:

$$\text{minimize}_{\mathbf{w},b} \quad \frac{1}{2}\mathbf{w}.\mathbf{w}$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1, \ \forall j$$

Rewrite constraints

One Lagrange multiplier per example

Lagrangian:

$$L(\mathbf{w}, \alpha) = \frac{1}{2}\mathbf{w}.\mathbf{w} - \sum_j \alpha_j \left[\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j - 1\right]$$
$$\alpha_j \geq 0, \ \forall j$$

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What's next?

- In next week's discussion, we will discuss:
  - Logistic Regression (Continued)
  - Naive Bayes, Linear Regression (Planned)

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Thank you!

Q & A