CSE4088 Introduction to Machine Learning

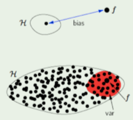
Linear Models II

Review of last time

- Bias and variance

Expected value of E_{out} w.r.t. $\mathcal{D}$

$= \text{bias} + \text{var}$

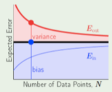


$g^{(\mathcal{D})}(\mathbf{x}) \rightarrow \bar{g}(\mathbf{x}) \rightarrow f(\mathbf{x})$

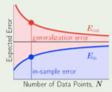
- Learning curves

How E_{in} and E_{out} vary with N

B-V:



VC:



- $N \propto$ "VC dimension"

Where we are

- Linear classification ✓
- Linear regression ✓
- Logistic regression
- Nonlinear transforms ✓

Nonlinear transforms

$$\mathbf{x} = (x_0, x_1, \cdots, x_d) \xrightarrow{\Phi} \mathbf{z} = (z_0, z_1, \cdots\cdots\cdots\cdots, z_{\tilde{d}})$$

Each $z_i = \phi_i(\mathbf{x})$ $\qquad \mathbf{z} = \Phi(\mathbf{x})$

Example: $\mathbf{z} = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$

Final hypothesis $g(\mathbf{x})$ in $\mathcal{X}$ space:

$\text{sign}\left(\tilde{\mathbf{w}}^{\mathsf{T}}\Phi(\mathbf{x})\right)$ or $\tilde{\mathbf{w}}^{\mathsf{T}}\Phi(\mathbf{x})$

The price we pay

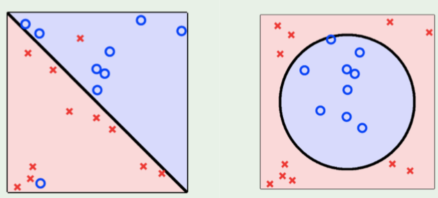
$$\mathbf{x} = (x_0, x_1, \cdots, x_d) \xrightarrow{\Phi} \mathbf{z} = (z_0, z_1, \cdots\cdots\cdots\cdots, z_{\tilde{d}})$$

$\downarrow \qquad\qquad \downarrow$

$\mathbf{w} \qquad\qquad \tilde{\mathbf{w}}$

$d_{\text{VC}} = d + 1 \qquad\qquad d_{\text{VC}} \leq \tilde{d} + 1$

Two non-seperable cases

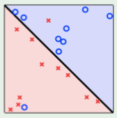


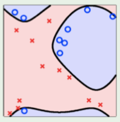
First case

Use a linear model in $\mathcal{X}$; accept $E_{\text{in}} > 0$

or

Insist on $E_{\text{in}} = 0$; go to high-dimensional $\mathcal{Z}$





We need a fourth order surface to have $E_{in} = 0$

This will not generalize well.

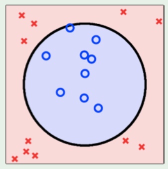
The second case

$\mathbf{z} = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$

Why not: $\mathbf{z} = (1, x_1^2, x_2^2)$

or better yet: $\mathbf{z} = (1, x_1^2 + x_2^2)$

or even: $\mathbf{z} = (x_1^2 + x_2^2 - 0.6)$



Lesson learned

Looking at the data *before* choosing the model can be hazardous to your E_{out}

Data snooping

Logistic Regression - Outline

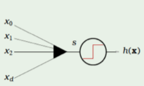
- The model
- Error measure
- Learning algorithm

A third linear model

$$s = \sum_{i=0}^{d} w_i x_i$$

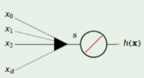
linear classification

$h(\mathbf{x}) = \text{sign}(s)$



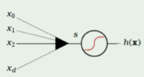
linear regression

$h(\mathbf{x}) = s$



logistic regression

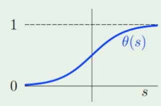
$h(\mathbf{x}) = \theta(s)$



The logistic function θ

The formula:

$$\theta(s) = \frac{e^s}{1 + e^s}$$



soft threshold: uncertainty

sigmoid: flattened out 's'

Probability interpretation

$h(\mathbf{x}) = \theta(s)$ is interpreted as a probability

Example. Prediction of heart attacks

Input $\mathbf{x}$: cholesterol level, age, weight, etc.

$\theta(s)$: probability of a heart attack

The signal $s = \mathbf{w}^{\intercal}\mathbf{x}$ "risk score"

Genuine probability

Data $(\mathbf{x}, y)$ with binary y, generated by a noisy target:

$$P(y \mid \mathbf{x}) = \begin{cases} f(\mathbf{x}) & \text{for } y = +1; \\ 1 - f(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

The target $f : \mathbb{R}^d \to [0, 1]$ is the probability

Learn $g(\mathbf{x}) = \theta(\mathbf{w}^{\intercal}\,\mathbf{x}) \approx f(\mathbf{x})$

Error measure

For each $(\mathbf{x}, y)$, y is generated by probability $f(\mathbf{x})$

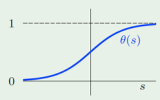
Plausible error measure based on **likelihood**:

If $h = f$, how likely to get y from $\mathbf{x}$?

$$P(y \mid \mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{for } y = +1; \\ 1 - h(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

Formula for likelihood

$$P(y \mid \mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{for } y = +1; \\ 1 - h(\mathbf{x}) & \text{for } y = -1. \end{cases}$$



Substitute $h(\mathbf{x}) = \theta(\mathbf{w}^{\intercal}\mathbf{x})$, noting $\theta(-s) = 1 - \theta(s)$

$P(y \mid \mathbf{x}) = \theta(y\ \mathbf{w}^{\intercal}\mathbf{x})$ Combine the two terms in the equation above.

Likelihood of $\mathcal{D} = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$ is The samples are generated independently

$$\prod_{n=1}^{N} P(y_n \mid \mathbf{x}_n) = \prod_{n=1}^{N} \theta(y_n \mathbf{w}^{\intercal}\mathbf{x}_n)$$

Maximizing the likelihood

Minimize
$$-\frac{1}{N} \ln\left(\prod_{n=1}^{N} \theta(y_n\ \mathbf{w}^{\intercal}\ \mathbf{x}_n)\right)$$

$$= \frac{1}{N} \sum_{n=1}^{N} \ln\left(\frac{1}{\theta(y_n\ \mathbf{w}^{\intercal}\ \mathbf{x}_n)}\right) \qquad \left[\theta(s) = \frac{1}{1 + e^{-s}}\right]$$

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \underbrace{\ln\left(1 + e^{-y_n \mathbf{w}^{\intercal}\mathbf{x}_n}\right)}_{e\left(h(\mathbf{x}_n), y_n\right)} \qquad \text{"cross-entropy" error}$$

Logistic Regression - Outline

- The model
- Error measure
- Learning algorithm

How to minimize E_{in}

For logistic regression,

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \ln\left(1 + e^{-y_n \mathbf{w}^{\mathsf{T}}\mathbf{x}_n}\right) \quad \longleftarrow \text{ iterative solution}$$

Compare to linear regression:

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}}\mathbf{x}_n - y_n)^2 \quad \longleftarrow \text{ closed-form solution}$$

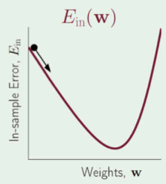
Iterative method: gradient descent

General method for nonlinear optimization

Start at $\mathbf{w}(0)$; take a step along steepest slope

Fixed step size: $\mathbf{w}(1) = \mathbf{w}(0) + \eta\,\hat{\mathbf{v}}$

What is the direction $\hat{\mathbf{v}}$?



Formula for the direction $\hat{\mathbf{v}}$

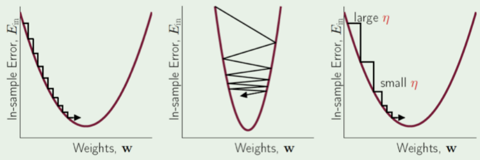
$$\begin{aligned}\Delta E_{\text{in}} &= E_{\text{in}}(\mathbf{w}(0) + \eta\hat{\mathbf{v}}) - E_{\text{in}}(\mathbf{w}(0)) \\ &= \eta \nabla E_{\text{in}}(\mathbf{w}(0))^{\mathsf{T}}\hat{\mathbf{v}} + O(\eta^2) \\ &\geq -\eta \|\nabla E_{\text{in}}(\mathbf{w}(0))\|\end{aligned}$$

Since $\hat{\mathbf{v}}$ is a unit vector,

$$\hat{\mathbf{v}} = -\frac{\nabla E_{\text{in}}(\mathbf{w}(0))}{\|\nabla E_{\text{in}}(\mathbf{w}(0))\|}$$

Fixed-size step?

How η affects the algorithm:



η too small | η too large | variable η – just right

η should increase with the slope

Easy implementation

Instead of

$$\Delta\mathbf{w} = \eta\,\hat{\mathbf{v}}$$

$$= -\eta \frac{\nabla E_{\text{in}}(\mathbf{w}(0))}{\|\nabla E_{\text{in}}(\mathbf{w}(0))\|}$$

Have

$$\Delta\mathbf{w} = -\eta\,\nabla E_{\text{in}}(\mathbf{w}(0))$$

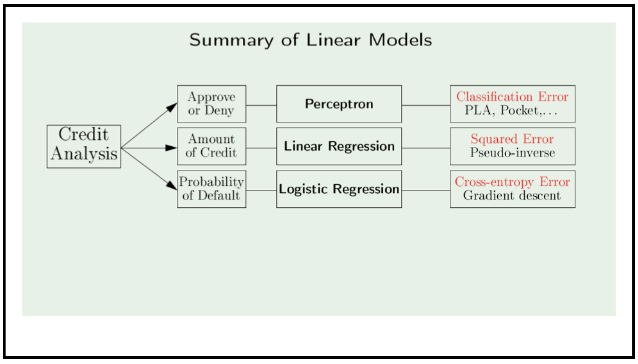
Fixed **learning rate** η

Logistic regression algorithm

1. Initialize the weights at $t = 0$ to $\mathbf{w}(0)$
2. **for** $t = 0, 1, 2, \ldots$ **do**
3. Compute the gradient

$$\nabla E_{\text{in}} = -\frac{1}{N}\sum_{n=1}^{N} \frac{y_n \mathbf{x}_n}{1 + e^{y_n \mathbf{w}^{\mathsf{T}}(t)\mathbf{x}_n}}$$

4. Update the weights: $\mathbf{w}(t+1) = \mathbf{w}(t) - \eta\nabla E_{\text{in}}$
5. Iterate to the next step until it is time to stop
6. Return the final weights $\mathbf{w}$


Summary of Linear Models
Credit Analysis
Approve or Deny
Amount of Credit
Probability of Default
Perceptron
Linear Regression
Logistic Regression
Classification Error
PLA, Pocket,...
Squared Error
Pseudo-inverse
Cross-entropy Error
Gradient descent