

Linear & Logistic Regression

Noa Lubin & Lior Sidi





Agenda

- Recap
- Regularization
- Linear Regression
- Logistic Regression
- Code
- Summary



Recap



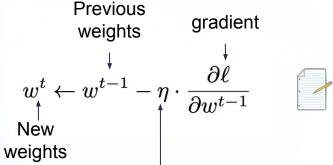


Gradient Descent

The idea of gradient descent is:

Take iterative steps to update parameters in the direction of the gradient

Previous



Step size / learning rate



Gradient Descent Training



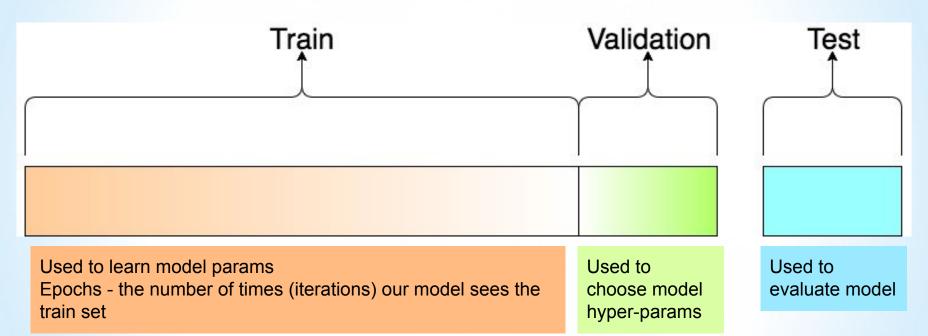
Algorithm 1 Gradient Descent Training

Input:

- Function $f(\mathbf{x}; \Theta)$ parameterized with parameters Θ .
- Training set of inputs $\mathbf{x_1}, \dots, \mathbf{x_n}$ and desired outputs $\mathbf{y_1}, \dots, \mathbf{y_n}$.
- Loss function L.
- 1: while stopping criteria not met do
- 2: Compute the loss $\mathcal{L}(\Theta) = \sum_{i} L(f(\mathbf{x_i}; \Theta), \mathbf{y_i})$ <-- slow! goes over all data.
- 3: $\hat{\mathbf{g}} \leftarrow \text{ gradients of } \mathcal{L}(\Theta)) \text{ w.r.t } \Theta$
- 4: $\Theta \leftarrow \Theta \eta_t \hat{\mathbf{g}}$
- 5: return Θ



Reminder:



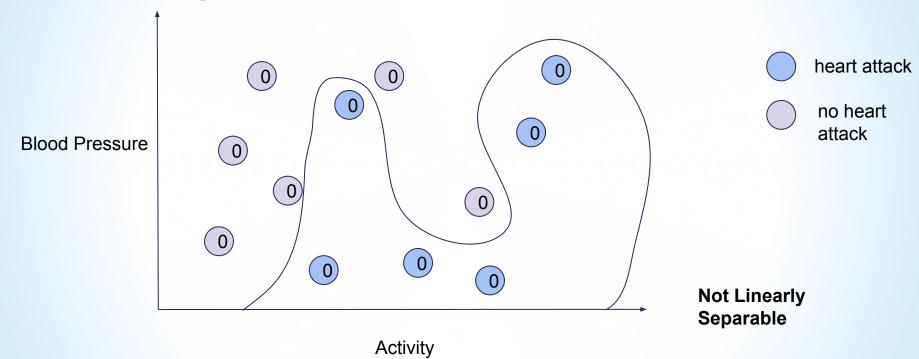


Regularization





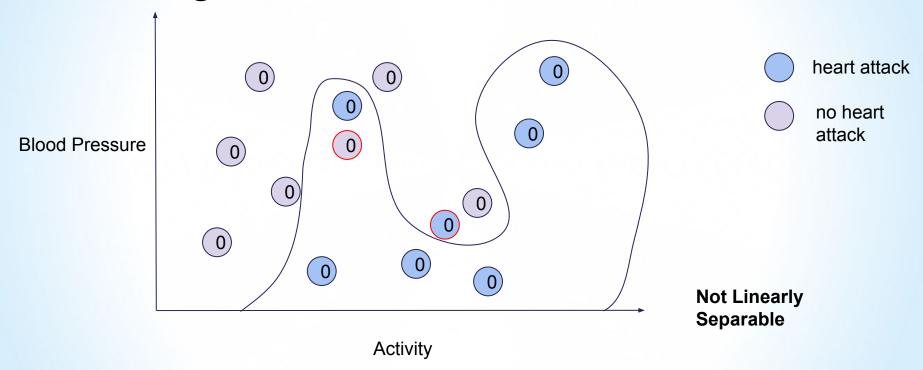
Overfitting



Loss = 0



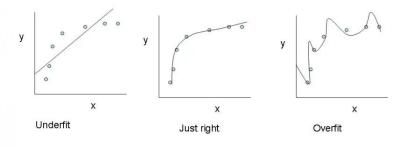
Overfitting - How Does it look on test set?



Loss = 0



Reminder: Underfitting & Overfitting





How to Handle Overfitting?

- Reduce the number of features
 - Manually select which features to keep
 - Automatic feature selection
- 2. Regularization
 - a. Keep all the features, but reduce the total weight of parameters θj
 - b. Regularization works well when we have a lot of slightly useful features
- 3. Normalization



Minimum Description Length Principle

This principle says we'll prefer a concise hypothesis over getting the entire training set right

$$w^* = \arg\min_{w} \frac{1}{m} \sum L(x_i, y_i; w) + \lambda \Omega(w)$$

High lambda - underfitting Low lambda - overfitting l_p norms can be used as regularizers

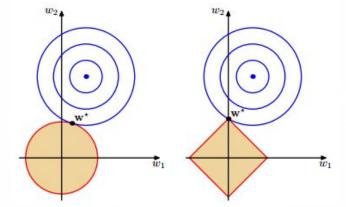


$$||\mathbf{w}||_2^2 = \sum_{d=1}^D w_d^2 \ ||\mathbf{w}||_1 = \sum_{d=1}^D |w_d| \ ||\mathbf{w}||_p = (\sum_{d=1}^D w_d^p)^{1/p}$$



lp norms

- Can be used as regularizers
- l2 norm: convex, smooth, easy to optimize
- l1 norm: encourages sparse w, convex, but not smooth at axis points
- p < 1: norm becomes non convex and hard to optimize

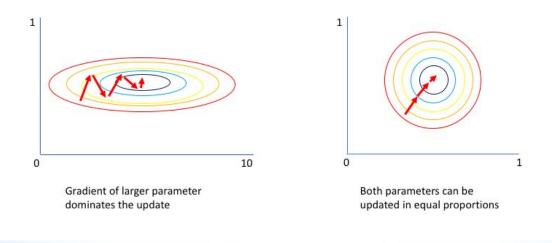




Normalization

Why is it important?

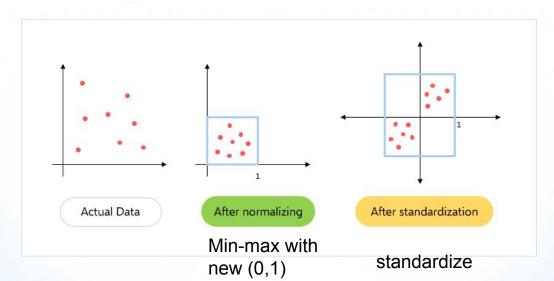
- Helps gradient descent to converge
- 2. We don't necessarily want large features to have larger impact
- 3. Some sort of regularization lower hypothesis search space





Normalization methods

Z-Score:
$$v' = \frac{v - mean_A}{stand_dev_A}$$

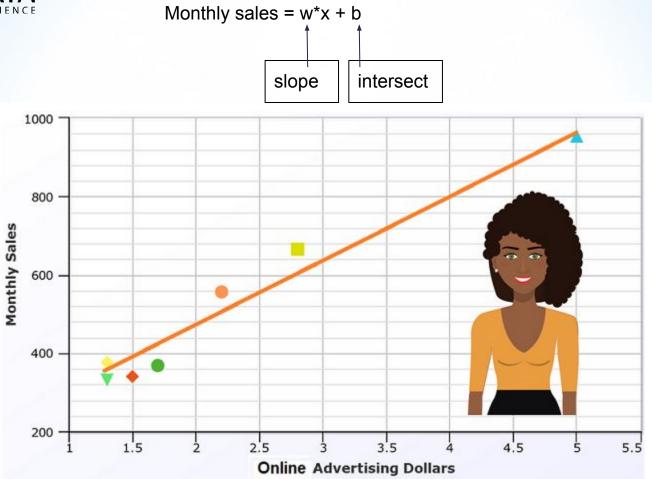




Linear Regression

$$L=rac{1}{2}\|(Xw-y)\|^2$$

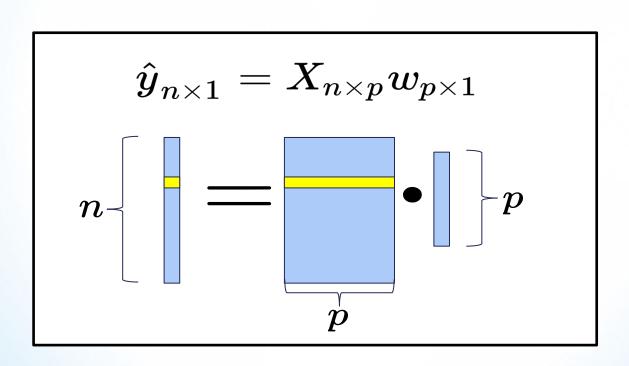






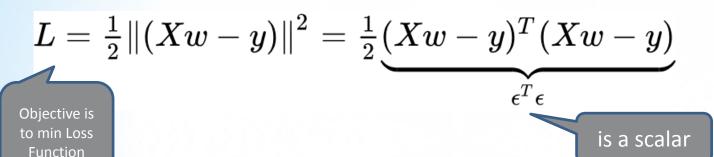
Matrix Form

1-padding for x





Residual Sum of Squares Loss





Residual Sum of Squares Loss

$$L=rac{1}{2}\|(Xw-y)\|^2=rac{1}{2}\underbrace{(Xw-y)^T(Xw-y)}_{\epsilon^T\epsilon}$$
 Objective is to min Loss Function

$$L=rac{1}{2}(w^TX^TXw-w^TX^Ty+y^Ty-y^TXw)$$



Common Matrix Derivatives

Notations

- O x is a scalar
- o x is a vector

Rule	Comments		
$(\mathbf{A}\mathbf{B})^T = \mathbf{B}^T \mathbf{A}^T$	order is reversed, everything is transposed		
$(\mathbf{a}^T \mathbf{B} \mathbf{c})^T = \mathbf{c}^T \mathbf{B}^T \mathbf{a}$	as above		
$\mathbf{a}^T\mathbf{b} = \mathbf{b}^T\mathbf{a}$	(the result is a scalar, and the transpose of a scalar is itself)		
$(\mathbf{A}+\mathbf{B})\mathbf{C}=\mathbf{AC}+\mathbf{BC}$	multiplication is distributive		
$(\mathbf{a} + \mathbf{b})^T \mathbf{C} = \mathbf{a}^T \mathbf{C} + \mathbf{b}^T \mathbf{C}$	as above, with vectors		
$AB \neq BA$	multiplication is not commutative		

Scalar derivative			Vector derivative		
f(x)	\rightarrow	$\frac{\mathrm{d}f}{\mathrm{d}x}$	$f(\mathbf{x})$	\rightarrow	$\frac{\mathrm{d}f}{\mathrm{d}\mathbf{x}}$
bx	\rightarrow	b	$\mathbf{x}^T \mathbf{B}$	\rightarrow	В
bx	\rightarrow	b	$\mathbf{x}^T\mathbf{b}$	\rightarrow	b
x^2	\rightarrow	2x	$\mathbf{x}^T\mathbf{x}$	\rightarrow	$2\mathbf{x}$
bx^2	\rightarrow	2bx	$\mathbf{x}^T \mathbf{B} \mathbf{x}$	\rightarrow	$2\mathbf{Bx}$



Residual Sum of Squares Loss

$$L=rac{1}{2}(w^TX^TXw-w^TX^Ty+y^Ty-y^TXw)$$

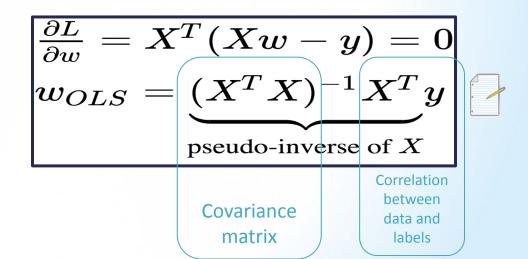
Scalar derivative		Vector derivative			
f(x)	\rightarrow	$\frac{\mathrm{d}f}{\mathrm{d}x}$	$f(\mathbf{x})$	\rightarrow	$\frac{\mathrm{d}f}{\mathrm{d}\mathbf{x}}$
bx	\rightarrow	b	$\mathbf{x}^T \mathbf{B}$	\rightarrow	В
bx	\rightarrow	b	$\mathbf{x}^T\mathbf{b}$	\rightarrow	b
x^2	\rightarrow	2x	$\mathbf{x}^T\mathbf{x}$	\rightarrow	$2\mathbf{x}$
bx^2	\rightarrow	2bx	$\mathbf{x}^T \mathbf{B} \mathbf{x}$	\rightarrow	2Bx





Closed Solution

$$egin{aligned} rac{\partial L}{\partial w} &= rac{1}{2}rac{\partial}{\partial w}(w^TX^TXw - w^TX^Ty + y^Ty - y^TXw) \ &= X^T(Xw - y) \end{aligned}$$





Why can't we always use a closed form solution?

Assumes linear independence

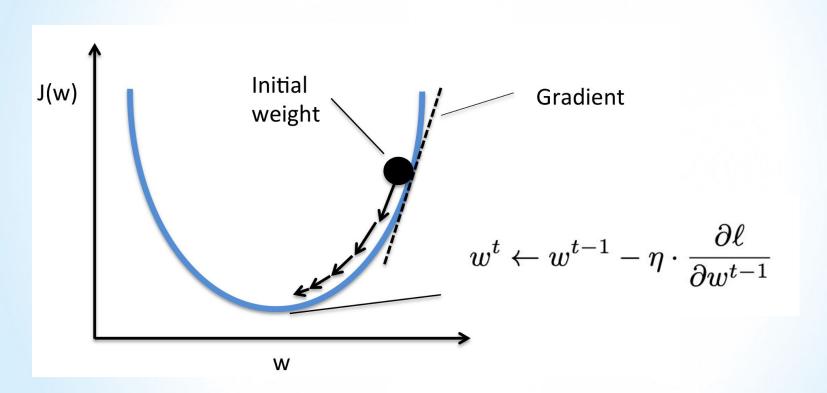
Doesn't necessarily exist - might be impossible to invert (X^TX)^-1

Solving inverse (X^TX)^-1 is computational expensive O(n^3)

Scale is an issue



Reminder: Gradient Descent for the Rescue



Gradient Descent for OLS (Ordinary Least Squares)

Let's plug the gradient into gradient descent formula

$$egin{aligned} rac{\partial L}{\partial w} &= X^T(Xw - y) \ w' &= \underbrace{w}_{ ext{old}} - \underbrace{\eta}_{ ext{learning rate}_{ ext{normalization}}} X^T(Xw - y) \end{aligned}$$



Weighted Least Squares (WLS)

- This can be used when some samples are more valuable than others (imbalance, noise)
- W is a diagonal matrix

$$egin{align} L &= rac{1}{2} \Big\| W^{rac{1}{2}}(Xw-y) \Big\|^2 \ \hat{w}_{WLS} &= (X^TWX)^{-1}X^TWy \end{aligned}$$

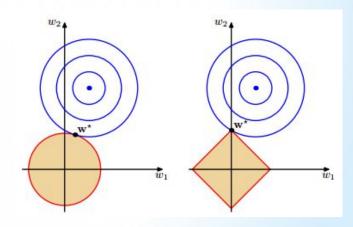


Reminder: Regularization

 l_p norms can be used as regularizers

$$||\mathbf{w}||_2^2 = \sum_{d=1}^D w_d^2$$

 $||\mathbf{w}||_1 = \sum_{d=1}^D |w_d|$
 $||\mathbf{w}||_p = (\sum_{d=1}^D w_d^p)^{1/p}$





Ridge: L₂ Loss Regularization for OLS

Minimize Objective function :

$$L = rac{1}{2} \|(Xw - y)\|^2 + \lambda \|w\|^2$$
OLS Model fitting term Regularization term

- Where λ is the regularization parameter
- We can easily modify both our gradient descent function and our closed-form solution to fit the new loss function.



Ridge: L₂ Loss Regularization

$$L=rac{1}{2}{\left\|\left(Xw-y
ight)
ight\|}^2+\lambda{\left\|w
ight\|}^2$$

$$rac{\partial L}{\partial w} = X^T(Xw-y) + \lambda w = 0$$
 $w_{ridge} = \underbrace{(X^TX + \lambda I\,)^{-1}X^T}_{ ext{pseudo-inverse of }X ext{ with diagonal loading}}_{ ext{pseudo-inverse of }X ext{ with diagonal loading}$



Lasso: L₁ Loss Regularization

OLS with L₁ penalty

$$w_{lasso} = \mathop{argmin}_{w} L = \underbrace{\frac{1}{2} \|(Xw - y)\|^2}_{ ext{OLS Loss}} + \lambda \underbrace{\|w\|}_{ ext{L1 Regularization}}$$
 $\|w\| = \sum_{k}^{p} \|w_k\|$

- Causes sparse weights
- Can be treated as "automatic feature selection"
- Harder to solve (solved using Coordinate Descent)



Elastic Net: Ridge and Lasso Combined

$$egin{aligned} w_{elastic} &= \mathop{argmin}_{w} L \ &= rac{1}{2} \|(Xw-y)\|^2 + \lambda_1 \left\|w
ight\| + \lambda_2 \left\|w
ight\|^2 \end{aligned}$$

Was found to be equivalent to SVM (will be discussed in SVM lecture)



Summary of Linear Regression

OLS	OLS + GD	Lasso	Ridge
Closed Solution	$rac{1}{2}\ (Xw-y)\ ^2$	$rac{1}{2}{\left\ {\left({Xw - y} ight)} ight\ ^2} + \lambda \left\ w ight\ $	$rac{1}{2}\ (Xw-y)\ ^2+\lambda\ w\ ^2$



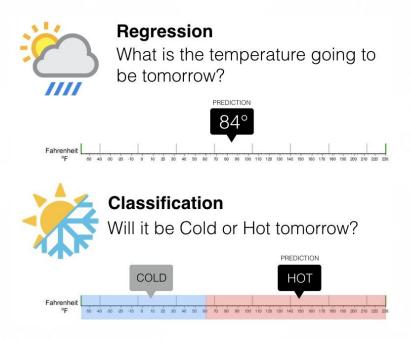
Logistic Regression

$$\ell_{ ext{cross-ent}} = -\sum_k \mathbf{y}_{[k]} \log \mathbf{\hat{y}}_{[k]}$$
 $\mathbf{\hat{y}} = \operatorname{softmax}(\mathbf{x}\mathbf{W} + \mathbf{b})$



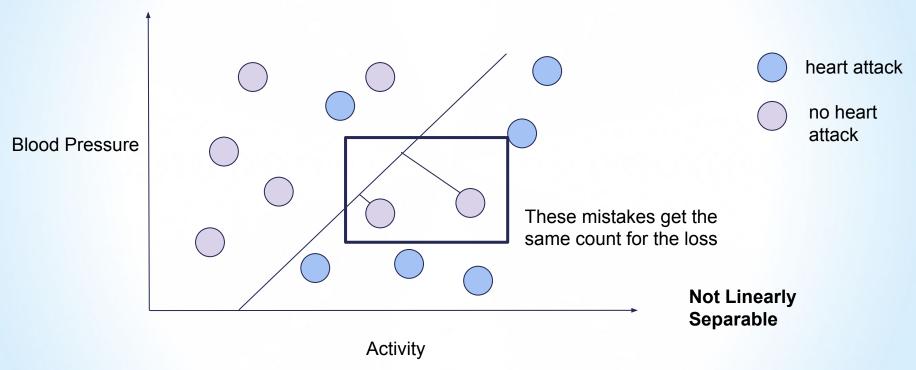


Classification vs Regression





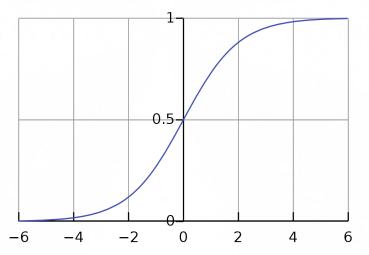
Why not use the 1-0 loss from before?





Can we do better? Sigmoid

$$\sigma(z_i)=rac{1}{1+e^{-z_i}}$$





Derivative of Sigmoid

$$\sigma(z_i)=rac{1}{1+e^{-z_i}}$$

What is the derivative of a sigmoid?

Where z=wx



Derivative of Sigmoid

$$egin{align} \sigma(z_i) &= rac{1}{1+e^{-z_i}} \ rac{\partial \sigma(z)}{\partial z} &= \sigma(z)(1-\sigma(z)) \ \end{aligned}$$

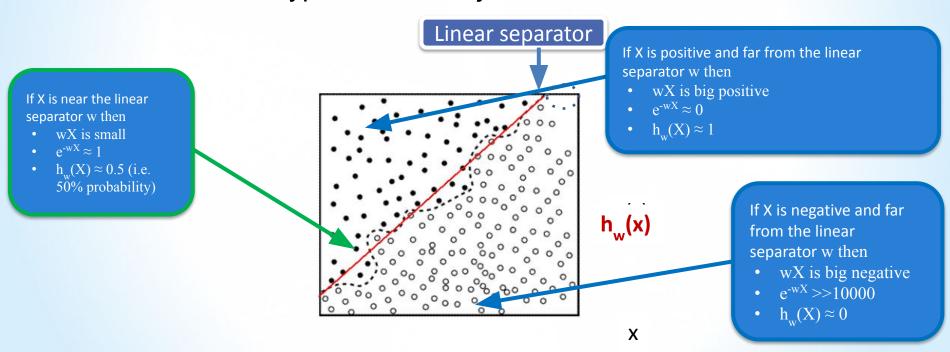
Where z=wx

$$\begin{split} \frac{\text{Sigmoid:}}{\left[\frac{1}{1+e^{-x}}\right]'} &= \frac{e^{-x}}{(1+e^{-x})^2} = \frac{1+e^{-x}-1}{(1+e^{-x})^2} = \frac{1+e^{-x}}{(1+e^{-x})^2} - \frac{1}{(1+e^{-x})^2} = \frac{1}{1+e^{-x}} - \frac{1}{(1+e^{-x})^2} \\ &= \frac{1}{1+e^{-x}} \left(1 - \frac{1}{1+e^{-x}}\right) = sigmoid*(1-sigmoid) \end{split}$$



Logistic Regression with Sigmoid Intuition

Different/Better Hypothesis & Objective





Another Intuition for Logistic Regression

The logistic regression model tries to predict the odds of an event:

$$\frac{p(X)}{1 - p(X)}$$

$$\frac{p(X)}{1 - p(X)} = e^{\beta^T X} = e^{\beta_1 X_1 + \dots + \beta_p X_p}$$

$$\log\left(\frac{p(X)}{1 - p(X)}\right) = \beta^T X$$

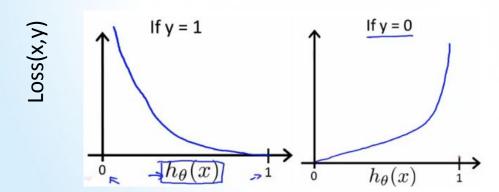
$$p(X) = \frac{\exp(\beta^T X)}{1 + \exp(\beta^T X)}$$



Cross Entropy Loss/Negative Log Likelihood

Let's define a loss for each observation based on a fix separator

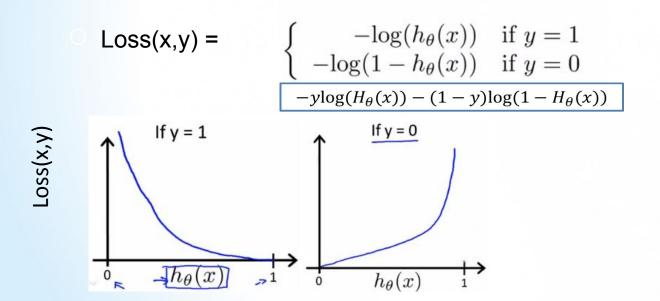
Loss(x,y) =
$$\begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1 \\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$





Cross Entropy Loss/Negative Log Likelihood

Let's define a loss for each observation based on a fix separator





LR Derivation Simplified

Optimize

$$G = y \cdot \log(h) + (1 - y) \cdot \log(1 - h)$$

Where

Derivation

$$\frac{dG}{d\theta} = \frac{dG}{dh} \frac{dh}{dz} \frac{dz}{d\theta}$$

 $h = 1/(1 + e^{-z}) \mid z(\theta) = x\theta$:

$$rac{dG}{\partial h} = rac{y}{h} - rac{1-y}{1-h} = rac{y-h}{h(1-h)}$$
 $rac{dh}{dz} = h(1-h)$ $rac{dz}{d heta} = x$

$$\frac{dh}{dz} = h(1-h)$$

Derivative of sigmoid

$$\frac{dG}{d\theta} = (y-h)x$$

Result



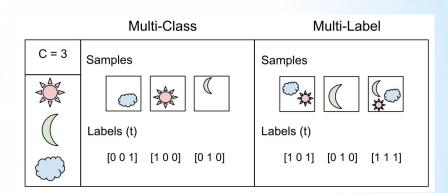
Reminder: Multi-Class & Multi-Label

Multiclass classification

Assigns a single class out of m possible classes (y output an integer between 1 and m)

Multilabel classification

Assign a 0 or 1 labels for each of the m possible classes (y output a binary vector of size m)





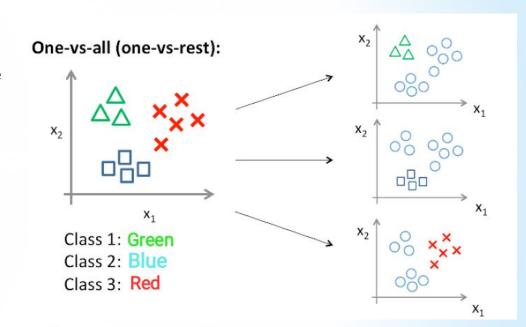
Heuristic Solutions to Multiclass Problems

One vs All (One vs Rest)

Training a single classifier per class, with the samples of that class as positive samples and all other samples as negatives - then choose the class with maximal confidence

One vs One

Train K (K – 1) / 2 binary classifiers, each receives the samples of a pair of classes from the original training set, and learn to distinguish these two classes. During prediction time, a voting scheme is applied





Cross Entropy Multiclass

$$egin{aligned} \ell_{ ext{cross-ent}} &= -\log \mathbf{\hat{y}}_{[t]} \ \ell_{ ext{cross-ent}} &= -\sum_k \mathbf{y}_{[k]} \log \mathbf{\hat{y}}_{[k]} \end{aligned}$$



Sigmoid for Multiclass (Softmax)

$$\sigma(z_i) = rac{1}{1+e^{-z_i}}$$

$$\operatorname{softmax}(\mathbf{v})_{[i]} = \frac{e^{\mathbf{v}_{[i]}}}{\sum_{i'} e^{\mathbf{v}_{[i']}}}$$



$$\hat{\mathbf{y}} = \operatorname{softmax}(\mathbf{x}\mathbf{W} + \mathbf{b})$$

$$e_{i]} = rac{e^{(\mathbf{x}\mathbf{W} + \mathbf{b})_{[i]}}}{\sum_{i} e^{(\mathbf{x}\mathbf{W} + \mathbf{b})_{[i]}}}$$

Cross Entropy Multiclass Derivative - Try this @ home

$$\begin{split} &\frac{\partial J(\theta)}{\partial \theta_{j}} = \frac{\partial}{\partial \theta_{j}} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log \left(h_{\theta} \left(x^{(i)} \right) \right) + (1 - y^{(i)}) \log \left(1 - h_{\theta} \left(x^{(i)} \right) \right) \right] \\ &= \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \frac{\partial}{\partial \theta_{j}} \log \left(h_{\theta} \left(x^{(i)} \right) \right) + (1 - y^{(i)}) \frac{\partial}{\partial \theta_{j}} \log \left(1 - h_{\theta} \left(x^{(i)} \right) \right) \right] \\ &= \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \frac{\partial}{\partial \theta_{j}} \log \left(h_{\theta} \left(x^{(i)} \right) \right) + (1 - y^{(i)}) \frac{\partial}{\partial \theta_{j}} \log \left(1 - h_{\theta} \left(x^{(i)} \right) \right) \right] \\ &= \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \frac{\partial}{\partial \theta_{j}} \sigma(\theta^{T} x^{(i)}) + (1 - y^{(i)}) \frac{\partial}{\partial \theta_{j}} (1 - \sigma(\theta^{T} x^{(i)})) \right] \\ &= \frac{-1}{\sigma^{i}} \sum_{i=1}^{m} \left[y^{(i)} \frac{\sigma(\theta^{T} x^{(i)}) (1 - \sigma(\theta^{T} x^{(i)})) \frac{\partial}{\partial \theta_{j}} (\theta^{T} x^{(i)})}{h_{\theta} \left(x^{(i)} \right)} - (1 - y^{(i)}) \frac{\sigma(\theta^{T} x^{(i)}) (1 - \sigma(\theta^{T} x^{(i)})) \frac{\partial}{\partial \theta_{j}} (\theta^{T} x^{(i)})}{1 - h_{\theta} \left(x^{(i)} \right)} \right] \\ &= \frac{-1}{\sigma^{i}} \sum_{i=1}^{m} \left[y^{(i)} \frac{h_{\theta} \left(x^{(i)} \right) (1 - h_{\theta} \left(x^{(i)} \right)) \frac{\partial}{\partial \theta_{j}} (\theta^{T} x^{(i)})}{h_{\theta} \left(x^{(i)} \right)} - (1 - y^{(i)}) \frac{h_{\theta} \left(x^{(i)} \right) (1 - h_{\theta} \left(x^{(i)} \right))}{2 - h_{\theta} \left(x^{(i)} \right)} \right] \\ &= \frac{-1}{\sigma^{i}} \sum_{i=1}^{m} \left[y^{i} - y^{i} h_{\theta} \left(x^{(i)} \right) - h_{\theta} \left(x^{(i)} \right) + y^{(i)} h_{\theta} \left(x^{(i)} \right) \right] x_{j}^{(i)} \\ &= \frac{1}{m} \sum_{i=1}^{m} \left[h_{\theta} \left(x^{(i)} \right) - y^{(i)} \right] x_{j}^{(i)} \end{aligned}$$



Other Loss Functions

- Hinge: $max(0, 1 ywx) \rightarrow You'll$ discuss this at SVM lecture
- Exponential loss
- C-loss
- ...



Explainability

ELI5 - Global explanation is the model W

month mar +1.170 +1.117 month_dec +0.968 education__illiterate +0.920 month oct +0.711 contact_cellular +0.619 month_sep job retired +0.615 +0.580 job_student +0.564 default no <BIAS> +0.528 +0.424 poutcome success +0.372 marital unknown +0.208 job unknown +0.201 housing no day_of_week__wed +0.193 +0.188housing_unknown ... 17 more positive 21 more negative ... -0.682 month_jul -0.761 month_may -0.798 month_aug -0.886month nov

Feature

y=1 top features

Weight?

Bank Marketing Data Set — <u>LINK</u>



Explainability

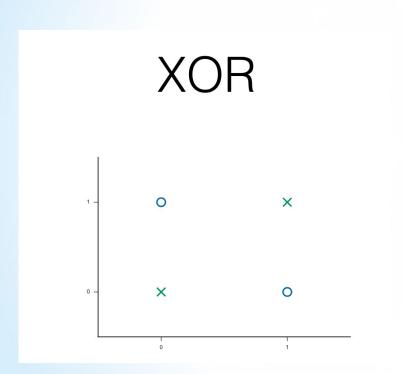
Local explanation is wx

y=1 (probability 0.961, score 3.203) top features

Contribution?	Feature	Value
+0.711	contactcellular	1.000
+0.564	defaultno	1.000
+0.528	<bias></bias>	1.000
+0.424	poutcome_success	1.000
+0.363	previous	2.000
+0.208	jobunknown	1.000
+0.193	day_of_weekwed	1.000
+0.188	marital_single	1.000
+0.156	loanno	1.000
+0.139	housing_yes	1.000
+0.129	age	27.000
+0.024	education_university.degree	1.000
-0.005	pdays	3.000
-0.146	monthjun	1.000
-0.271	campaign	4.000



Can we build a linear model for XOR?



$$(0,0) \cdot \mathbf{w} + b < 0$$

$$(0,1) \cdot \mathbf{w} + b \ge 0$$

$$(1,0) \cdot \mathbf{w} + b \ge 0$$

$$(1,1) \cdot \mathbf{w} + b < 0$$

$$\mathbf{W} = \mathbf{\hat{x}}$$



Can we build a linear model for XOR?

Linear Models will underfit xor, we need non-linearity which can be achieved:

- * data pre-processing
- * kernels
- * adding non-linearity to the model



Code





Let's Think About This Together

- 1. What are the main hyper-parameters?
- Can it work for multi-class data (relevant only for logistic)?
- 3. How does it handle categorical data?
- 4. How does it handle missing data?
- 5. Is it sensitive to outliers?
- 6. What if some features are correlated?
- 7. Is it prone to overfitting?
- 8. Is it Interpretable?
- 9. Can it be parallelized?
- 10. Speed of training
- 11. Speed of prediction



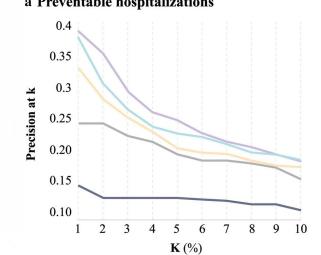
Let's Think About This Together

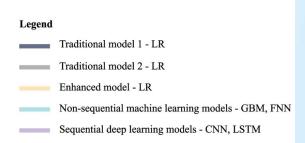
- What are the main hyper-parameters? Optimizer: LR, stopping criteria, initial weights, epochs, regularization lambda
- 2. Can it work for multi-class data (relevant only for logistic)? Yes
- 3. How does it handle categorical data? We need to make it numeric
- 4. How does it handle missing data? No
- 5. Is it sensitive to outliers? Yes
- 6. What if some features are correlated? Doesn't handle well
- 7. Is it prone to overfitting? Regularization
- 8. Is it Interpretable? Yes
- 9. Can it be parallelized? Not off the shelf
- 10. Speed of training depends on optimizer and hyper-params
- 11. Speed of prediction linear



Congestive Heart Failure

Comparison of deep learning with traditional models to predict preventable acute care use and spending among heart failure patients







Summary





Summary

	Linear Regression	Logistic Regression
Target Type	Regression	Classification
Loss	$rac{1}{2}\ (Xw-y)\ ^2$	$\ell_{ ext{cross-ent}} = -\sum_k \mathbf{y}_{[k]} \log \mathbf{\hat{y}}_{[k]}$
		$\mathbf{\hat{y}} = \operatorname{softmax}(\mathbf{xW} + \mathbf{b})$



Pros and Cons

Pros	Cons
 Fast Simple Explainable 	 Can't handle missing data - needs imputation Categorical data needs translation to numeric Assumption of linear relations Sensitivity to correlated features