

Linear Regression: MSE (mean-squared error) objective function: $J_p(\vec{w}, b) = \frac{1}{N} \sum_{i=1}^N (y^{(i)} - (\vec{w}^T \vec{x}^{(i)} + b))^2$

- gradient descent: $\vec{g} \leftarrow \nabla_{\vec{\theta}} J(\vec{\theta}) = \frac{1}{N} \sum_{i=1}^N (\vec{\theta}^T \vec{x}^{(i)} - y^{(i)}) \vec{x}^{(i)}$, $\vec{\theta} \leftarrow \vec{\theta} - \eta \vec{g}$ per iteration. (MN)

→ local optimisation algo \Leftrightarrow converge to local min of J exists \Leftrightarrow GD/LR globally convergent. (soln exists, may not be unique)

minimizing MSE: $\nabla J(\vec{\theta}) = 0 \Leftrightarrow X^T X \vec{\theta} = X^T y \Leftrightarrow \text{lstsq}(X, y)$ \Leftrightarrow find argmin $\|\vec{\theta}\|$ s.t. normal eqn satisfied

→ soln unique $\Leftrightarrow N$ (# examples) \geq # of LI features (e.g. 3D \Rightarrow 1 or 2 LI features if on line/plane)

Stochastic Gradient Descent: $\vec{\theta} \leftarrow \vec{\theta} - \eta \nabla_{\vec{\theta}} J^{(i)}(\vec{\theta})$, $i \sim U[1, N]$ or shuffle $[1, N]$

- epoch = single pass through training data (GD \Leftrightarrow 1 update/epoch, SGD \Leftrightarrow N updates)

	# steps to convergence	compute/step
GD	$O(\log(1/\epsilon))$	$O(NM)$
SGD	$O(1/\epsilon)$	$O(NM)$

* LHP under assumptions
 ↓ learning rate \Rightarrow SGD behaves like GD
 both initial training MSE large due to uninformed init.

MLE: $\vec{\theta}^{MLE} = \arg\max_{\vec{\theta}} \prod_{i=1}^N p(y^{(i)} | \vec{x}^{(i)}, \vec{\theta}) = \arg\max_{\vec{\theta}} p(D|\vec{\theta})$, $\vec{\theta}^{MAP} = \arg\max_{\vec{\theta}} p(D|\vec{\theta})p(\vec{\theta})$

[recall] (online) perceptron: $\hat{y} = \text{sign}(\vec{\theta}^T \vec{x}^{(i)})$, if misclassified, $\vec{\theta} \leftarrow \vec{\theta} + y^{(i)} \vec{x}^{(i)}$

Logistic Regression: $p(y | \vec{x}, \vec{\theta}) = y = 1 \Leftrightarrow \sigma(\vec{\theta}^T \vec{x})$, $y = 0 \Leftrightarrow 1 - \sigma(\vec{\theta}^T \vec{x})$

- $\mathcal{L}(\vec{\theta}) = -\sum_{i=1}^N \log p(y^{(i)} | \vec{x}^{(i)}, \vec{\theta})$, $J(\vec{\theta}) = -\frac{\mathcal{L}(\vec{\theta})}{N} \Rightarrow \frac{\partial J(\vec{\theta})}{\partial \vec{\theta}} = -(y^{(i)} - \sigma(\vec{\theta}^T \vec{x})) \vec{x}^{(i)}$

- prediction: $\hat{y} = 1 \Leftrightarrow \sigma(\vec{\theta}^T \vec{x}) \geq 0.5$ $\uparrow \vec{\theta} \leftarrow \vec{\theta} + \delta(y^{(i)} - \sigma(\vec{\theta}^T \vec{x})) \vec{x}^{(i)}$ always updated.

Regularization: prevent overfitting (idea: Occam's razor): $\hat{\vec{\theta}} = \arg\min_{\vec{\theta}} J(\vec{\theta}) + \lambda R(\vec{\theta})$

L1/Lasso: $\|\vec{\theta}\|_1 = \sum_{i=1}^M |\theta_i|$, L2/Ridge: $\|\vec{\theta}\|_2 = \sqrt{\sum_{i=1}^M \theta_i^2}$

→ true function classifier training error used to choose $h \in \mathcal{H}$ fit model params.

Learning Theory: true error rate $R(h) = \mathbb{E}_{x \sim p} [\mathbb{I}(c^*(x) \neq h(x))]$ is unknown * validation error to choose \mathcal{H} (hyperparameters)

empirical risk/training error $\hat{R}(h) = \mathbb{E}_{x \sim D} [\mathbb{I}(y^{(i)} \neq h(x^{(i)}))]$

→ c^* may be unachievable, but achievable (true) risk minimizer $h^* = \arg\min_{h \in \mathcal{H}} R(h)$ unknown

only know empirical risk minimizer $\hat{h} = \arg\min_{h \in \mathcal{H}} \hat{R}(h)$. overfitting = $\hat{R}(h) - R(h)$

PAC (Probably Approximately Correct) criterion: $P(|R(h) - \hat{R}(h)| \leq \epsilon) \geq 1 - \delta \forall h \in \mathcal{H}$

→ ϵ is diff between true & empirical risk, δ is probability of "failure"

ERM (empirical risk minimization) on \mathcal{H} with M training ex.

→ sample complexity = M needed in order to satisfy PAC for given ϵ, δ → finite if $|\mathcal{H}| < \infty$, infinite if $|\mathcal{H}| = \infty$.

→ Bayesian view: $\vec{\theta}$ is RV, described by prior & posterior, MAP find estimator that $\rightarrow \vec{\theta}$ quickly, even for noisy data

Frequentist: $\vec{\theta}$ as a constant, (regularized) MLE, consistency/convergence rates/robustness

→ regularized MLE \equiv MAP if regularizer = log(prior), but justification different.

→ MAP estimate = mode of posterior; β -distribution $\propto \theta^{\alpha-1} (1-\theta)^{\beta-1}$ → α moves mass to $\theta=1$, $\beta \rightarrow \theta=0$

$\vec{x} \Leftrightarrow 6 \times 1$, $\vec{x}^{(1)}$ is bias (1 added) \leftarrow weights α is $3 \times (6+1)$

$\vec{a} = \vec{w}^T \vec{x}^{(1)} \Leftrightarrow a_j = \alpha_j + \sum_{i=1}^6 \alpha_{j,i} x_i \forall 1 \leq j \leq 3$

→ # of neurons in hidden layer is 3

$\vec{z} = \text{ReLU}(\vec{a}) = \max(0, \vec{a})$, \vec{z} is $3 \times 1 \Leftrightarrow$ alternative sigmoid $\sigma(u) = \frac{1}{1+e^{-u}}$

→ $\vec{z}^{4 \times (3+1)}$ → prepend 1 to 1st entry of \vec{z} $\rightarrow \frac{\partial \mathcal{L}}{\partial \vec{a}} = \mathbb{I}[\vec{a} > 0] \rightarrow \sigma'(u) = \sigma(u)(1-\sigma(u))$

$\vec{b} = \vec{\beta}^T \vec{z} \Leftrightarrow 4 \times 1$ * if $\vec{\beta}$ 1-row of non-zero values, \vec{b} reducible to layer \vec{w}

→ softmax(\vec{b}) = $\frac{\exp(b_k)}{\sum_{l=1}^4 \exp(b_l)}$ single neuron (ie. all d-1 neurons have output 0)

→ $\frac{\partial \mathcal{L}}{\partial b_k} = \hat{y}_k (\mathbb{I}[k=2] - \hat{y}_k)$ \leftarrow 1-hot vector

$\mathcal{L}(\vec{y}, \vec{\hat{y}}) = -\sum_{i=1}^4 y_i \ln(\hat{y}_i) \rightarrow \frac{\partial \mathcal{L}}{\partial \hat{y}_i} = -\frac{y_i}{\hat{y}_i}$ & $\sum_{i=1}^4 y_i = 1$

→ LINEAR: $\vec{x} \rightarrow \vec{z} \rightarrow \vec{y}$ used to calculate $\frac{\partial \mathcal{L}}{\partial \vec{\alpha}}$

fwd: return $\vec{z} @ \vec{x}^{(1)} \leftarrow$ cache $\vec{x}^{(1)}$ \leftarrow no bias bc. $\beta_{k,0}$ are not affected by values of α

bck: $\frac{\partial \mathcal{L}}{\partial \vec{w}} = \frac{\partial \mathcal{L}}{\partial \vec{z}} \vec{x}^T$ (np.outer($dz, \vec{x}^{(1)}$)), return $\frac{\partial \mathcal{L}}{\partial \vec{z}} = (\vec{w}^*)^T \frac{\partial \mathcal{L}}{\partial \vec{z}} \rightarrow$ step: $\vec{w} \leftarrow \vec{w} + \eta \frac{\partial \mathcal{L}}{\partial \vec{w}}$

→ ReLU: fwd cache $\max(0, \vec{x})$, bck $\frac{\partial \mathcal{L}}{\partial \text{in}} = \mathbb{I}[\text{out} > 0] * (\text{cache} > 0)$

Sigmoid: fwd cache $1/(1+\exp(-x))$, bck $\frac{\partial \mathcal{L}}{\partial \text{in}} = \frac{\partial \mathcal{L}}{\partial \text{out}} \text{cache} (1-\text{cache})$

→ Softmax Cross Entropy: fwd return $(\vec{y}, -\ln \hat{y}_k)$, bck $y_k = [0, \dots, 1, \dots, 0]$ for $\frac{\partial \mathcal{L}}{\partial b_k}$

→ if separate: $\mathcal{L}_b = \mathcal{L}_g(\text{diag}(\vec{y}) - \vec{y} \vec{y}^T) + \mathcal{L} = -\vec{y}^T \ln \vec{y}$, $\mathcal{L}_g = -\sum_{j=1}^4 g_{j,k} \leftarrow 1$

① for finite \mathcal{H} s.t. $c^* \in \mathcal{H}$ (realizable), and arbitrary distribution p^* , if # labelled training data p^*

$M \geq \frac{1}{\epsilon} (\ln(|\mathcal{H}|) + \ln(\frac{1}{\delta}))$ then with prob $\geq 1 - \delta$, $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$

\leftarrow if k h with $R(h) > \epsilon$ * union bound + $\ln(1+\epsilon) \leq \epsilon$

$\hat{P} \equiv E = \text{event } \exists h \in \mathcal{H} \text{ with } \hat{R}(h) = 0, R(h) > \epsilon, \text{ then } P(E) < \delta$

$P(E) < k(1-\epsilon)^M \leq |\mathcal{H}|(1-\epsilon)^M \Rightarrow \ln P(E) < \ln |\mathcal{H}| + M \ln(1-\epsilon)$ \leftarrow boolean variables $\Rightarrow |\mathcal{H}| = 3^d \rightarrow \frac{1}{2}, 0, \text{ absent}$

→ Cor: given training data x & S s.t. $|S| = M$, all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \frac{1}{M} (\ln |\mathcal{H}| + \ln(\frac{1}{\delta}))$

② for finite \mathcal{H} and arbitrary dist. p^* , if # labelled training dpts satisfies $R(h) < \epsilon$ u.p. at least $1 - \delta$

$M \geq \frac{1}{2\epsilon^2} (\ln |\mathcal{H}| + \ln(\frac{1}{\delta}))$, then up at least $1 - \delta$, all $h \in \mathcal{H}$ satisfy $|R(h) - \hat{R}(h)| \leq \epsilon$

→ Cor: ... s.t. $|S| = M$, all $h \in \mathcal{H}$ have $R(h) \leq \hat{R}(h) + \sqrt{\frac{1}{2M} (\ln |\mathcal{H}| + \ln(\frac{1}{\delta}))}$ u.p. at least $1 - \delta$.

Def: \mathcal{H} shatters set of pts if it can classify them all possible ways

Sauer's lemma: sps $S_H(M) = 2^d$ for $M \leq d$, but $S_H(d+1) < 2^{d+1}$, then $S_H(M) = O(M^d)$

→ VC(\mathcal{H}) = size of largest set \mathcal{H} can shatter (\exists d pts... \nexists d+1 pts...)

→ halfspaces in d dimensions: VC = $d+1$ → so $|\mathcal{H}| \rightarrow S_H(M)$ (thms)

if $S_H(M) = 2^M \forall M$, not learnable/can memo at any $|D|$, if bounded, can memo at most d .

Algorithm 1 SGD

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1: Initialize  $\theta^{(0)}$ 
2:
3:
4:  $s = 0$ 
5: for  $t = 1, 2, \dots, T$  do
6:   for  $i \in \text{shuffle}(1, \dots, N)$  do
7:     Select the next training point  $(x_i, y_i)$ 
8:     Compute the gradient  $g^{(s)} = \nabla J_i(\theta^{(s-1)})$ 
9:     Update parameters  $\theta^{(s)} = \theta^{(s-1)} - \eta g^{(s)}$ 
10:    Increment time step  $s = s + 1$ 
11:  Evaluate average training loss  $J(\theta) = \frac{1}{n} \sum_{i=1}^n J_i(\theta)$ 
12: return  $\theta^{(s)}$ 

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Algorithm 1 Mini-Batch SGD

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1: Initialize  $\theta^{(0)}$ 
2: Divide examples  $\{1, \dots, N\}$  randomly into batches  $\{I_1, \dots, I_B\}$ 
3: where  $\bigcup_{b=1}^B I_b = \{1, \dots, N\}$  and  $\bigcap_{b=1}^B I_b = \emptyset$ 
4:  $s = 0$ 
5: for  $t = 1, 2, \dots, T$  do
6:   for  $b = 1, 2, \dots, B$  do
7:     Select the next batch  $I_b$ , where  $m = |I_b|$ 
8:     Compute the gradient  $g^{(s)} = \frac{1}{m} \sum_{i \in I_b} \nabla J_i(\theta^{(s)})$ 
9:     Update parameters  $\theta^{(s)} = \theta^{(s-1)} - \eta g^{(s)}$ 
10:    Increment time step  $s = s + 1$ 
11:  Evaluate average training loss  $J(\theta) = \frac{1}{n} \sum_{i=1}^n J_i(\theta)$ 
12: return  $\theta^{(s)}$ 

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Convexity: $f: \mathbb{R}^D \rightarrow \mathbb{R}$ is convex if $\forall \mathbf{x}^{(1)}, \mathbf{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c < 1$, $f(c\mathbf{x}^{(1)} + (1-c)\mathbf{x}^{(2)}) \leq cf(\mathbf{x}^{(1)}) + (1-c)f(\mathbf{x}^{(2)})$, linear functions are convex, ax^2 concave for $a < 0$

- MSE, MAE are convex, strictly convex iff \mathbf{x} has full column rank (otherwise infinite minimizers in nullspace); adding strictly convex regulariser makes both strictly convex
- Convex \rightarrow converge to global minima which might not exist (e.g. e^x) (exist for MSE/MAE)

Don't use test error in making model selection decisions!

Matrix multiplication for $[M \times N][N \times P] \in O(MNP)$, matrix inverse in $O(N^3)$

Conditional likelihood: iid samples $D = \{x^{(i)}, y^{(i)}\}$ from a pair of RVs (unlike likelihood function with single X RV with pmf $p(x | \theta)$), Y discrete with pmf $p(y | x, \theta)$

Forward Computation:

Given: $y = \exp(xz) + \frac{xz}{\log(x)} + \frac{\sin(\log(x))}{xz} = f(x, z)$

Computation Graph:

Backward Computation:

False positive rate FPR = FP / N
False negative rate FNR = FN / P
Positive predictive value/precision = TP / PP
Negative predictive value = TN / PN
True positive rate/recall = TP / P
Accuracy = (TP + TN) / (TP + FN + FP + TN)

Given: $x=2, z=3$

$a = xz$
 $b = \log(x)$
 $c = \sin(b)$
 $d = \exp(a)$
 $e = a/b$
 $f = c/a$
 $y = d + e + f$

Backward Computation:

$\frac{\partial y}{\partial x} = \frac{\partial d}{\partial x} + \frac{\partial e}{\partial x} + \frac{\partial f}{\partial x}$
 $\frac{\partial d}{\partial x} = \frac{\partial \exp(xz)}{\partial x} = \exp(xz) \cdot z = d \cdot z$
 $\frac{\partial e}{\partial x} = \frac{\partial (a/b)}{\partial x} = \frac{1}{b} \cdot \frac{\partial a}{\partial x} - \frac{a}{b^2} \cdot \frac{\partial b}{\partial x}$
 $\frac{\partial f}{\partial x} = \frac{\partial (c/a)}{\partial x} = \frac{1}{a} \cdot \frac{\partial c}{\partial x} - \frac{c}{a^2} \cdot \frac{\partial a}{\partial x}$

Achieving fairness: (1) pre-processing data, (2) additional constraints during training, (3) post-processing predictions – premise for 1+2: if def of fairness satisfied in training data, then most models will preserve that relationship. A protected label, X applicant data, Y pred

1. **Independence** (selection rate parity): $h(X, A) \perp A$, prop of accepted applicants same for all genders (adjust penalty for predicting +ve in class till we get parity/use diff threshold), permits laziness (alw pred +1)/susceptible to adversaries (admit some randomly)

- Prediction rate is the same across values of A , $P(h = 1 | A = a_1) = P(h = 1 | A = a_2)$

2. **Separation** (FPR = FNR): $h(X, A) \perp A | Y$, all good/bad applicants accepted with same prob rgdless of A , perpetuate existing bias (only access to target var thru historical data)

- Among individuals of the same true label, $P(h = 1 | Y, A)$, classifier independent of A

3. **Sufficiency** (PPV = NPV): $Y \perp A | h(X, A)$, among people who receive the same prediction, the actual probability of being positive is the same across groups, $P(Y = 1 | h, A)$ independent of A (i.e., the info contained in $h(X, A)$ is sufficient, A becomes irrelevant)

If baseline rates of label across both values of A equal, then $Y \perp A$, both S 's can be achieved.