EXPERIMENTAL METHODS

treatment/indie variable what we are able to control
outcome/dependent variable what we observe
stratification i.e. stratify by demographic vars before splitting into ctrl groups
double-blind even experimenters don't know who is placebo
observational study experiment not randomizable
control variable i.e. income level on education
confounding variable influences both treatment and outcome variables

HYPOTHESIS TESTING WITH HYPERGEOMETRIC

aka **Fisher's exact test**

does drug help? we assume H_0 is $\mu_1 = \mu_2$ so we use Hypergeometric distribution to check what is probability of drawing these numbers of deaths between study and control group under H_0.

p-value: $\sum_{i=0}^{39} P_{H_0}(T = i)$

pro doesn't assume knowledge of true value in ctrl group
con assumes knowledge of margins

z-test if we know the true value of σ

t-test if we estimate $\widehat{\sigma}$: $\frac{\overline{X}_n}{\frac{\widehat{\sigma}}{\sqrt{n}}} \sim t_{n-1}$

PYTHON MISC

convert row vector into column vector

```
Y = Y.reshape(-1,1)
```

sigmoid

```
from scipy.stats import logistic
logistic.cdf(x)
```

TODO

Linear regression
* multivariable
* remove insignificant variables

LOAD CSV DATA

```
import pandas as pd

data = pd.read_csv('gamma-ray.csv')
```

PANDAS MISC

get first row

```
df.iloc[0]
```

LIKELIHOOD RATIO TEST (POISSON)

```
from scipy import stats

n = 1
d = 1
for row in data.data.iterrows():
    G_i = row["count"]
    t_i = row["seconds"]
    lambda_i = G_i/t_i
    n *= stats.poisson.pmf(G_i, lambda_mle)
    d *= stats.poisson.pmf(G_i, lambda_i)

test_statistic = -2*np.log(n/d)
test_statistic
```

QQ PLOTS

here we were trying to figure out if we should apply a log transformation to some fields

```
stats.probplot(data[key], dist="norm", plot=plt)
plt.show()
stats.probplot(np.log(data[key]), dist="norm", plot=plt)
plt.show()
```

LINEAR CLASSIFIERS

boundary line: $\theta \cdot x + \theta_0 = 0$

$\theta \cdot x$ is positive if x is on the right side of the decision boundary

PERCEPTRON

$y^{(i)} \in \{-1, 1\}$

training error: $\varepsilon(\theta, \theta_0) = \frac{1}{n} \sum 1\left\{y^{(i)}\left(\theta \cdot x^{(i)} + \theta_0\right) \leq 0\right\}$

algorithm

$\theta = \vec{0}$
for t = 1...T
  for i = 1...n
    if $y^{(i)}\left(\theta \cdot x^{(i)} + \theta_0\right) \leq 0$ then
      $\theta = \theta + y^{(i)} x^{(i)}$
      $\theta_0 = \theta_0 + y^{(i)}$

REGULARIZATION

we want large boundaries: $\vdots$ | $\vdots$
where $\vdots$ are $\theta \cdot x^{(i)} + \theta_0 = \{1, -1\}$ and | is $\theta \cdot x^{(i)} + \theta_0 = 0$
· prevents overfitting
· the bigger $\|\theta\|$ the faster (= shorter distance) these reach -1 and 1
· we can control the margins distance with $\|\theta\|$

signed distance

$\gamma_i = y^{(i)} \frac{\theta \cdot x^{(i)} + \theta_0}{\|\theta\|} = \frac{1}{\|\theta\|}$ or $-\frac{1}{\|\theta\|}$

to maximise $\frac{1}{\|\theta\|}$ we minimise $\frac{1}{2}\|\theta\|^2$

hinge loss

$$Loss_h(z) = Loss_h(y^{(i)}(\theta \cdot x^{(i)} + \theta_0)) = max(0, 1 - y^{(i)}(\theta * x^{(i)} + \theta_0))$$
$$= \begin{cases} 0 & \text{if } z \geq 1 \quad \text{correct side, outside margins} \\ 1 - z & \text{if } z < 1 \end{cases}$$

hinge loss improves by moving θ towards example

objective

$J(\theta, \theta_0) = \frac{1}{n} \sum Loss_h\left(y^{(i)}\left(\theta \cdot x^{(i)} + \theta_0\right)\right) + \frac{\lambda}{2}\|\theta\|^2$

where λ is regularisation loss and minimising that term increases margins

$\rightarrow$ by minimising J we balance maximising margins and minimising loss

gradient descent

$\theta \Leftarrow \theta - \eta \nabla J(\theta)$

SOLVING QUADRATIC

if linearly separable and don't allow any errors, can solve quadratic:

$\Rightarrow J(\theta, \theta_0) = \frac{1}{2}\|\theta\|^2$

STOCHASTIC GRADIENT DESCENT

update: sample i at random

decreasing learning rate $\eta_T = \frac{1}{1+T}$

$$\theta \Leftarrow \theta - \eta_T \nabla_\theta \left[Loss_h\left(y^{(i)} \theta \cdot x^{(i)}\right) + \frac{\lambda}{2}\|\theta\|^2\right]$$

$$= \theta\left[\begin{cases} 0 & \text{if } Loss_h = 0 \\ -y^{(i)} \cdot x^{(i)} & \text{if } Loss_h > 0 \end{cases} + \lambda\theta\right]$$

LINEAR REGRESSION

empirical risk

$R_n(\theta) = \frac{1}{n} \sum \frac{\left(y^{(t)} - \theta x^{(t)}\right)^2}{2}$

small deviations less penalised than large ones

$\nabla_\theta R_n(\theta) = -\left(y^{(i)} - \theta x^{(t)}\right) \cdot x^{(t)}$

gradient descent

$\theta = 0$
  for:
    random $t = \{1...n\}$ # stochastic, could also loop
      $\theta = \theta + \eta_k\left(y^{(t)} - \theta \cdot x^{(t)}\right) \cdot x^{(t)}$

with $\eta_k = \frac{1}{1+k}$

NONLINEAR CLASSIFICATION

not linearly separable $\Rightarrow$ map x to higher dimension

kernels

i.e. $K(x, x') = \phi(x) \cdot \phi(X') = (x \cdot x') + (x \cdot x')^2$

where $\phi(x) = \left(x_1, x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2\right)^T$

$\Rightarrow$ dot product is cheap to compute

COLLABORATIVE FILTERING

assumes X has low rank

$J(u, v) = \sum_{a,i \in D} \frac{(Y_{ai} - u_a v_i)^2}{2} + \frac{\lambda}{2}\sum^n u_a^2 + \frac{\lambda}{2}\sum^m v_i^2$

$X = \begin{bmatrix} \text{user1rating1} & \text{user1rating2} \\ \text{user2rating1} & \text{user2rating2} \end{bmatrix} = u \cdot v^T$

$\Rightarrow$ u: user's rating tendency
$\Rightarrow$ v: info about movie

alternating projections set v, optimise u, set u...
continue until local convergence
(exercise link)

KERNEL PERCEPTRON

$\theta = 0$
for $i = 1...n$
  if $y^{(i)} \ \theta \cdot \phi\left(x^{(i)}\right) \ \leq 0$
    $\theta \Leftarrow \theta + y^{(i)}\phi\left(x^{(i)}\right)$

$\theta \cdot \phi\left(x^{(i)}\right) = \sum_j^n \alpha_j y^{(j)} \phi\left(x^{(j)}\right)\phi\left(x^{(i)}\right)$

where α_j is nb of mistakes made on j^{th} example

we can then rewrite the perceptron algorithm without having to transform $x \Rightarrow \phi(x)$ anymore

$\theta = 0$
for $i = 1...n$
  if $y^{(i)} \sum_j^n \alpha_j y^{(j)} K\left(x^{(j)}, x^{(i)}\right) \leq 0$
    $\alpha_i = \alpha_i + 1$

kernel composition

· $f: \mathbb{R}^d \rightarrow R$ and $K(x, x')$
$\widetilde{K}(x, x') = f(x)K(x, x')f(x')$
· $K(x, x') = K_1(x, x') + K_2(x, x')$
· $K(x, x') = K_1(x, x') + K_2(x, x')$

radial basis kernel

$K(x, x') = \exp\left(-\frac{1}{2}\|x - x'\|^2\right)$

$\Rightarrow$ correctly classifies every point
$\Rightarrow$ radial in `phi(x) space

graph classification
look at number of bends in figure to determine dimension

K-NEAREST NEIGHBOURS

$\widehat{Y}_{ai} = \frac{1}{K} \sum_{b \in \text{KNN}(a,i)} Y_{bi}$

or weigh by similarity

$\widehat{Y}_{ai} = \frac{\sum_{b \in \text{KNN}(a,i)} sim(a, b) Y_{bi}}{\sum_{b \in \text{KNN}} sim(a, b)}$

euclidian distance $\|x_a - x_b\|$
cosine similarity $\cos(\theta) = \frac{x_a \cdot x_b}{\|x_a\|\|x_b\|}$

limitations my combination of tastes maybe uncommon

ACTIVATION FUNCTIONS

ReLU $f(z) = \max(0, z)$
tanh $f(z) = \tanh(z)$
linear $f(z) = z$

MISC

$\vec{a} \cdot \vec{b} = \sum a_i b_i$
$a \cdot a = \|a\|^2$
$\theta_z \cdot Ax = \theta_z^T Ax = \left(A^T \theta_z\right) \cdot x$

distance from point to line
$d = \frac{|\theta \cdot x + \theta_0|}{\|\theta\|}$

derivative of norm squared
$\left(\|h(x)\|^2\right)' = 2h(x)h'(x)$

derivative $[y(\theta \cdot x)]' = yx$
because we derive for each θ_i

L1 norm $\|w\|_1 = \sum_i^n |w_i|$

L2 norm $\|w\|_2 = \sqrt{\sum_i^n w_i^2}$

cosine similarity
$\cos\left(x^{(i),x^{(j)}}\right) = \frac{x^{(i)} \cdot x^{(j)}}{\|x^{(i)}\|\|x^{(j)}\|}$

euclidean distance
$dist\left(x^{(i)}, x^{(j)}\right) = \|x^{(i)} - x^{(j)}\|$

DEEP LEARNING

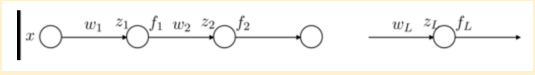
· intermediate layer is like feature representation: "learning ϕ"
· activation layer acts like linear classifier

backpropagation
compute partial derivatives using chain rule to do gradient descent

$$w_1 \Leftarrow w_1 - \eta\left(\frac{\delta \text{Loss}}{\delta w_1}\right)$$

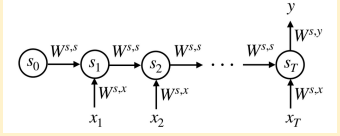
$$\frac{\delta \text{Loss}}{\delta w_1} = \frac{\delta \text{Loss}}{\delta f_1} \cdot \frac{\delta f_1}{\delta z_1} \cdot \frac{\delta z_1}{\delta w_1}$$

risks are vanishing or exploding gradients with long chains



RNN

· same params for each layer
· variable number of layers
⇒ encodes sentences



$$s_t = \tanh(W^{s,s} s_{t-1} + W^{s,x} x_t)$$

RNN have some gradient issues

gating network
in default RNN we overwrite s_t but sometimes it's useful to retain control over what's overwritten at each step

$$g_t = \text{sigmoid}(W^{g,s} s_{t-1} + W^{g,x} x_t)$$
$$s_t = (1 - g_t) \odot s_{t-1} + g_t \odot \tanh(W^{s,s} s_{t-1} + W^{s,x} x_t)$$

where $\odot$ is element-wise multiplication

$(1 - g_t)$: $\begin{pmatrix}0\\1\\0\end{pmatrix} \rightarrow \begin{pmatrix}1\\0\\1\end{pmatrix}$ i.e. g_t is use to control what we retain from previous layer

MARKOV MODELS

<beg> w_1 w_2 w_3 <end>
w_0 w_L

$$P(w_1, ..., w_L) = P(w_1 \mid w_0)...P(w_L \mid w_{L-1})$$

with $P(w' \mid w) = \dfrac{\text{count}(w, w')}{\sum_{\tilde{w}} \text{count}(w, \tilde{w})}$

RNNs for sequences
variable history

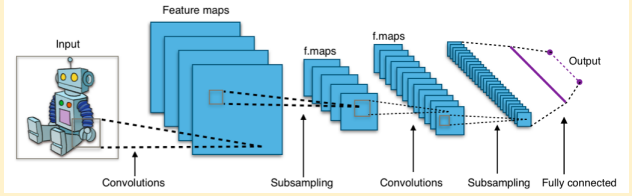
ϕ(word) $\vdots X^W \vdots^{S_t} X \vdots p$
s_{t-1} $\vdots X$

i.e. we're feeding the previous state as input to the next

CNN

convolution
· classify by small patches
· slide over input
· use the same weights for each patch to build feature map

pooling (subsampling)
· stores *if* there's an activation for feature in that area
· stride



cross-correlation/convolution
we don't actually need to flip $g(t)$ as we would with convolution, because we're learning the filter, the values are just flipped

1d $f \odot g(t) = \sum f(T) g(T + t)$

md $f \odot g(x, y) = \sum_{T_1} \sum_{T_2} f(T_1, T_2) g(T_1 + x, T_2 + y)$

K-MEANS

1) randomly assign $z^{(1)}...z^{(2)}$
2) iterate
  a) assign x to closest z

$$\text{Cost}\left(z^{(1)}...z^{(k)}\right) = \sum_{i=1}^{n} \min_{j=1...k} \left\|x^{(i)} - z^{(j)}\right\|^2$$

  b) given $C_1...C_k$ find best rep. z in each C

$$\text{Cost}(C_1...C_k) = \min_{z^{(1)}...z^{(k)}} \sum_{j=1}^{k} \sum_{i \in C_j} \left\|x^{(i)} - z^{(j)}\right\|^2$$

problems with K-means
· points are not in set of Xs
· $(\text{euclidean distance})^2$ only
· K-means is $O(n \cdot k \cdot d)$ for one update step (2)

find best z_j for C_j

$$\frac{\delta}{\delta z_j} \sum_{i \in C_j} \left\|x^{(i)} - z^{(j)}\right\|^2 = 0$$

$$z^{(j)} = \frac{\sum x^{(i)}}{|C_j|}$$

where $|C_j|$ is size of C_j

impact of init
· init matters
· we can end up with undesirable convergence

K-MEDIANS

Like K-means but with medians. Compute median in each single dimension in the Manhattan distance formulation (see ex.)

K-MEDOIDS

1) pick init $z^{(i)}...z^{(j)}$ from points X
2) iterate until no change in cost
  a) for $i = 1...n$

$$C_j = \left\{i : z^{(j)} \text{ is closest to } x^{(i)}\right\}$$

  b) pick the most central $x^{(i)}$ in C_j to be $z^{(j)}$

for $j = 1...k$

$$z_j = \left\{x^{(i)}...x^{(n)} : \sum_{i \in C_j} dist\left(x^{(i)}, z^{(j)}\right) \text{ is minimal}\right\}$$

· same idea as K-means but z_j is in x and can use any distance measure
· K-medoids is $O\left(n^2 \cdot k \cdot d\right)$ for update step (2)

⚠ step 2 gets executed even if no change and cost, and order we cycle in matters and can update the medoid (see ex.)

GENERATIVE MODELS

$p(w \mid \theta) = \theta w$: probability of generating word w given all possibilities`

probability of generating doc D

$$p(D \mid \theta) = \prod_{i=1}^{n} \theta_{w_i} = \prod_{w \in W} \theta_w^{\text{count}(w)}\Big)$$

MLE

$$\max\ P(D \mid \theta) \rightarrow \sum_{w \in W} \text{count}(w) \log(\theta_w)$$

$$\Rightarrow \tilde{\theta}_w = \frac{\text{count}(w)}{\sum_{w' \in W} \text{count}(w')}$$

prediction
essentially acts as a linear classifier through origin

$$\log \frac{p(D \mid \theta^+)}{p(D \mid \theta^-)} = \begin{cases} \geq 0 & + \\ < 0 & - \end{cases}$$

prior, posterior, likelihood
for when we have same prior knowledge of document classification

$$P(y = + \mid D) = \frac{P(D \mid \theta^+) P(y = +)}{P(D)}$$

⇒ linear classifier with offset influenced by prior

⚠ N-1 params in multinomial (i.e. remember the binomial uses 1 param for two values)

GAUSSIAN GENERATIVE MODELS

$X \mid \mu, \sigma^2 \sim N\left(\mu, \sigma^2\right)$

want to find μ and σ^2 that give highest likelihood to training data.

$\Rightarrow \frac{\delta l_n}{\delta \mu} = 0$ and $\frac{\delta l_n}{\delta \sigma^2} = 0$

$\widehat{\mu} = \frac{1}{n}\sum^{n} x^{(i)}$ and $\widehat{\sigma^2} = \frac{1}{nd}\sum^{n} \left\| x^{(i)} - \mu \right\|^2$

MIXTURE MODELS

mixture components K: $N\left(x, \mu_j, \sigma_j^2\right)$

mixture weights $p_1 ... p_k \quad \sum p_j = 1$

$\theta = p_1 ... p_k, \mu_1 ... \mu_k, \sigma_1^2 ... \sigma_k^2$

$p(x \mid \theta) = \sum_{j=1}^{k} p_j N\left(x, \mu_j, \sigma_j^2\right)$

$p(S_n \mid \theta) = \prod_{i=1}^{n} \prod_{j=1}^{k} p_j N\left(x, \mu_j, \sigma_j^2\right)$

EM algorithm

"random" init of $\theta: \mu^{(i)}, \sigma^{(i)}, p_i$
init matters for speed and outcome

· converges locally
· good idea to use k-means for init

expectation step

$p(j \mid i) = \frac{p_j N\left(x_i, \mu_j, \sigma_j^2 I\right)}{p(x \mid \theta)}$

$\Rightarrow$ probability that point i in cluster j

$\Rightarrow \quad p(x \mid \theta) = \sum_{j=1}^{k} p_j N\left(x_i, \mu_j, \sigma_j^2 I\right)$

maximisation step
re-estimate parameters, (nb: cluster j, point i)

$\widehat{n}_j = \sum_{i=1}^{n} p(j \mid i)$

$\hat{p}_j = \frac{\widehat{n}_j}{n}$

$\widehat{\mu}_j = \frac{1}{\widehat{n}_j} \sum_{i=1}^{n} p(j \mid i) x^{(i)}$

$\widehat{\sigma}_j^2 = \frac{1}{\widehat{n}_j d} \sum_{i=1}^{n} p(j \mid i) \left\| x^{(i)} - \mu^{(j)} \right\|^2$

MARKOV DECISION PROCESS

· states $s \in S$
· actions $a \in A$
· action dependent on transition probabilities

$T(s, a, s') = P(s' \mid a, s)$
$\sum_{s' \in S} T(s, a, s') = 1$

$R(s, a, s')$: reward for starting s, doing a, ending s'

UTILITY FUNCTIONS

finite horizon (not important)

count reward for next n steps: $U(s_0 ... s_n) = \sum^{n} R(s_i)$

infinite horizon/discounted reward

$U(s_0 ... s_n) = \sum_{k=0}^{\infty} Y^k R(s_k) \leq \frac{R_{\max}}{1 - \gamma}$

value function

$V^\star(s)$: expected reward if agent acts optimally starting at s

$\pi: S \to A$: assigns action $\pi(s)$ to state s
optimal policy $\pi^\star$ assigns action at every state that maximises expected utility

$Q^\star(s, a)$: expected reward starting at s, taking action a and acting optimally

BELLMAN EQUATIONS

$V^\star(s) = \max_a Q^\star(s, a) = Q^\star(s, \pi^\star(s))$

$Q^\star(s, a) = \sum_{s'} T(s, a, s')[R(s, a, s') + \gamma V^\star(s')]$

VALUE ITERATION ALGORITHM

$V_k^\star(s) \to_{k \to \infty} V(s)$

· init: $V_0^\star(s) = 0$
· iterate until $V_k^\star(s) \approx V_{k+1}^\star(s) \forall s$

$V_{k+1}^\star = \max_a \left[\sum_{s'} T(s, a, s') \left[R(s, a, s') + \gamma V_k^\star(s') \right] \right]$

· compute $Q^\star(s, a)$

then $\pi^\star(s) = arg \max_a Q^\star(s, a)$

Q-VALUE ITERATION

same as above but with Q and the update is:

$Q_{k+1}^\star = \sum_{s'} T(s, a, s') \left[R(s, a, s') + \gamma \max_{a'} Q_k^\star(s', a') \right]$

$\Rightarrow$ we're summing over all possible states we may land in

RL

typically won't have T and R ahead of time

Q-value iteration
want to calculate estimates for Q but don't have T and R.
we'll use **exponential running average** to get estimates for $Q(s, a)$:

$Q_{i+1}(s, a) = \alpha \cdot \text{sample} + (1 - \alpha) Q_i(s, a)$
sample: $R(s, a, s') + \gamma \max_{a'} Q_i(s', a')$

1) **initialisation** $Q(s, a) = 0 \forall a$

2) **iterate until convergence**

a) collect samples: s,a,s',R(s,a,s')

b) $Q_{i+1}(s, a) = \alpha \left[R(s, a, s') + \gamma \max_{a'} Q_i(s', a') \right] + (1 - \alpha) Q_i(s, a)$

ε greedy

balance exploration and exploitation

· random action w.p. ε
· best current action w.p. $(1 - \varepsilon)$

ε should decay over time