## 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 $\sigma$

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

## LOAD CSV DATA

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

optional header=None and index_col

## 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
```

## LINEAR REGRESSION

**add first column of 1s**

```
X.insert(0, "label", np.ones((100,1)))
```

**LSE/Bayes estimator**

```
beta = np.linalg.inv(X.T@X)@X.T@y
# y is row vector, X is rows for sample
```

## WELCH T TEST (ex.)

*find features that are significantly different between two sample populations*

```
result = stats.ttest_ind(data_aml, data_all, axis=1,
equal_var=False, nan_policy='raise',
alternative='two-sided')
```

## MULTIPLE HYPOTHESES TESTING CORRECTIONS

**holm-bonferroni**

```
pvalues = sorted(result.pvalue)
count = 0
alpha = 0.05

for i, v in enumerate(pvalues):
    if v <= alpha/(len(pvalues) - i):
        count += 1

count
```

**bonferroni-hochberg**

```
pvalues = sorted(result.pvalue)
alpha = 0.05

for i, v in enumerate(pvalues):
    if v <= (i+1)/len(pvalues) * alpha:
        continue
    else:
        break

print(i)
```

## T TEST TO FIND UNNECESSARY LIN.REG. PARAMS (theory.)

```
N = len(y) # nb of data points
p = len(X[0]) # dimension of a sample feature vector
var_hat = (np.linalg.norm(y - X@beta)**2)/(N - p)
sigma_hat = np.sqrt(var_hat)
beta_cov = np.linalg.inv(X.T@X)
# T statistics
Ts = beta/(sigma_hat*np.sqrt(np.diagonal(beta_cov)))
pvalues = 2*scipy.stats.t.sf(np.abs(Ts), (N - p))
```

## PYTHON MISC

convert row vector into column vector

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

**sigmoid**

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

**build feature matrix X from individual arrays**

```
X = np.vstack((np.ones((1,30)), A, B)).T
```

## PANDAS MISC

**get first row**

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

**get first 10 columns**

```
df.iloc[:, 0:10]
```

**iterate rows**

```
for index, row in data.iterrows():
  print(row["seconds"])
```

**mean (of each row, over columns)**

```
df.mean(axis=1)
```

## 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()
```

## GRADIENT DESCENT

```
def gradient_descent(X, y, step_size, precision):
    beta = np.zeros((X.shape[1], 1))
    losses = []

    def loss(beta, X, y):
        return float(np.sum(np.square(y - X@beta)))

    def loss_grad(beta, X, y):
        return (y - X@beta).T@X

    while True:
        last_loss = loss(beta, X, y)
        beta += step_size * loss_grad(beta, X, y).T
        this_loss = loss(beta, X, y)
        if abs(last_loss - this_loss) <= precision:
            break

    return beta

gradient_descent(X, y, 0.005, 10**(-6))
```

## MLE (ex.)

derive MLE by hand, then implement as code

## 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**

```
θ = $\vec{0}$
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: ⋮ | ⋮

where ⋮ 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**

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

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

**hinge loss**

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

hinge loss improves by moving $\theta$ 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 $\lambda$ 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** $\eta_T = \frac{1}{1 + T}$

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

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

## 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**

```
θ = 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

```
θ = 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 $\alpha_j$ 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

```
θ = 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 $\theta_i$

**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**

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

## DEEP LEARNING

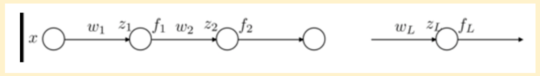
· intermediate layer is like feature representation: "learning $\phi$"
· activation layer acts like linear classifier

**backpropagation**
compute partial derivatives using chain rule to do gradient descent

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

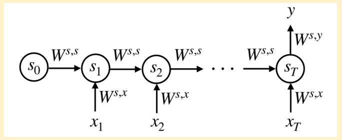
$$\frac{\delta\text{Loss}}{\delta w_1} = \frac{\delta\text{Loss}}{\delta f_1}\cdot\frac{\delta f_1}{\delta z_1}\cdot\frac{\delta z_1}{\delta w_1}$$

risks are vanishing or exploding gradients with long chains



## RNN

· same params for each layer
· variable number of layers
$\Rightarrow$ 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>
$w_0$ $w_L$

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

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

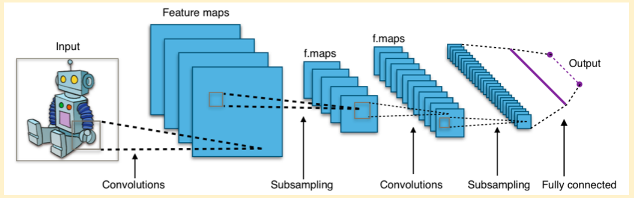
**RNNs for sequences**
variable history

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

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 $z^{(1)}\ldots z^{(2)}$
2) iterate
  a) assign x to closest z

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

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

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

**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 $z^{(i)}\ldots z^{(j)}$ from points X
2) iterate until no change in cost
  a) for $i = 1\ldots n$
    $C_j = \left\{i : z^{(j)} \text{ is closest to } x^{(i)}\right\}$

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

    for $j = 1\ldots k$

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

· 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**

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

**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

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

$\Rightarrow$ 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 $\mu$ and $\sigma^2$ 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** $p_1 \ldots p_k$ $\sum p_j = 1$

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

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

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

## 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

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

**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: $U(s_0 \ldots s_n) = \sum^{n} R(s_i)$

**infinite horizon/discounted reward**

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

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

**$\varepsilon$ greedy**

balance exploration and exploitation

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

$\varepsilon$ should decay over time