#### COMP90051

# Workshop Week 12

## About the Workshops

- □ 7 sessions in total
  - ☐ Tue 12:00-13:00 AH211
  - ☐ Tue 12:00-13:00 AH108 \*
  - ☐ Tue 13:00-14:00 AH210
  - ☐ Tue 16:15-17:15 AH109
  - ☐ Tue 17:15-18:15 AH236 \*
  - ☐ Tue 18:15-19:15 AH236 \*
  - ☐ Fri 14:15-15:15 AH211

#### About the Workshops

Homepage

https://trevorcohn.github.io/comp90051-2017/workshops

☐ Solutions will be released on next Friday (a week later).

# Syllabus

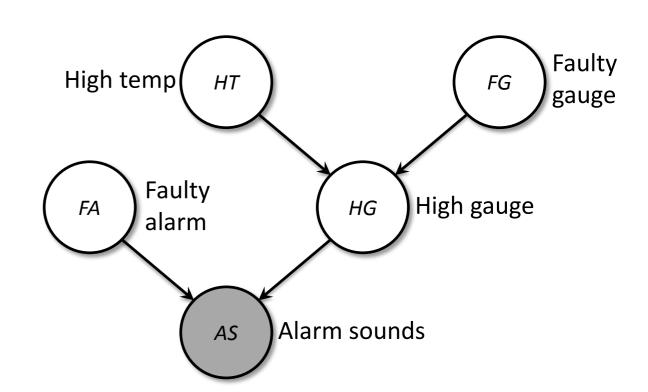
1	Introduction; Probability theory	Probabilistic models; Parameter fitting	
2	Linear regression; Introduction to regularization	Logistic regression; Basis expansion	
3	Optimization; Regularization	Perceptron	
4	Backpropagation	CNNs; Auto-encoders	
5	Hard-margin SVMs	Soft-margin SVMs	
6	Kernel methods	Ensemble Learning	
7	Clustering	EM algorithm	
8	Principal component analysis; Multidimensional Scaling	Manifold Learning; Spectral clustering	
9	Bayesian inference (uncertainty, updating)	Bayesian inference (conjugate priors)	
10	PGMs, fundamentals	PGMs, independence	
11	PGMs, inference	PGMs, EM algorithm	<b>←</b>
12	PGMs, HMMs & message passing	Subject review	

#### Outline

- ☐ Review the lecture, background knowledge, etc.
  - ☐ Elimination algorithm
  - Sampling method
  - EM algorithm

# Nuclear power plant

- Alarm sounds; meltdown?!
- $\Pr(HT|AS = t) = \frac{\Pr(HT, AS = t)}{\Pr(AS = t)}$ =  $\frac{\sum_{FG, HG, FA} \Pr(AS = t, FA, HG, FG, HT)}{\sum_{FG, HG, FA, HT'} \Pr(AS = t, FA, HR, FG, HT')}$



Numerator (denominator similar)

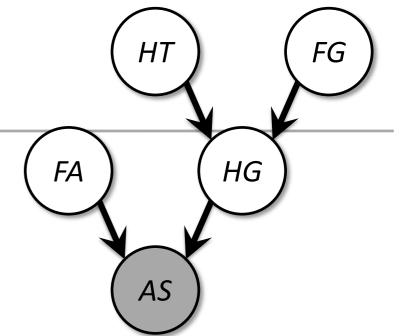
expanding out sums, joint summing once over 25 table

$$= \sum_{FG} \sum_{HG} \sum_{FA} \Pr(HT) \Pr(HG|HT,FG) \Pr(FG) \Pr(AS = t|FA,HG) \Pr(FA)$$

distributing the sums as far down as possible summing over several smaller tables

$$= \Pr(HT) \sum_{FG} \Pr(FG) \sum_{HG} \Pr(HG|HT, FG) \sum_{FA} \Pr(FA) \Pr(AS = t|FA, HG)$$

# To calculate P(HT|AS = 1)



Joint

P(AS, FA, HG, HT, FG) = P(AS|FA, HG)P(FA)P(HG|HT, FG)P(HT)P(FG)

- $\square \text{ Step 1. } P(HT|AS=1) \propto P(AS=1,HT)$
- $\square \operatorname{Step} 2. P(AS = 1, HT) = \sum_{FG, HG, FA} P(AS = 1, FA, HG, HT, FG)$
- ☐ Step 3. Normalize  $P(AS = 1, HT) \rightarrow P(HT|AS = 1)$

- $\square P(AS = 1, HT)$  has two numbers
  - $\square P(AS = 1, HT = 0) \text{ and } P(AS = 1, HT = 1)$
  - can be calculated together

☐ We will first see a Naive way to calculate them

#### Define some tables

```
HG
table_FG = np.asarray([0.1, 0.9]) \leftarrow P(FG)
table_HT = np.asarray([0.2, 0.8]) \leftarrow P(HT)
table_FA = np.asarray([0.3, 0.7]) \leftarrow P(FA)
                                                     AS
table_HG_HT_FG = np.empty((2, 2, 2)) \leftarrow P(HG|HT,FG)
table_HG_HT_FG[:, 0, 0] = [0.35, 0.65]
table HG HT FG[:, 0, 1] = [0.25, 0.75]
table_HG_HT_FG[:, 1, 0] = [0.15, 0.85]
table HG HT FG[:, 1, 1] = [0.05, 0.95]
table_AS_FA_HG = np.empty((2, 2, 2)) \leftarrow P(AS|FA, HG)
table_AS_FA_HG[:, 0, 0] = [0.45, 0.55]
table_AS_FA_HG[:, 0, 1] = [0.55, 0.45]
table AS FA HG[:, 1, 0] = [0.65, 0.35]
table AS FA HG[:, 1, 1] = [0.75, 0.25]
```

```
P(AS = 1, HT) = \sum_{FG, HG, FA} P(AS = 1, FA, HG, HT, FG)
                                                         HG
AS = 1
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
             for FA in [0, 1]:
                 prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                                  table HG HT FG[HG, HT, FG] *
                                  table FA[FA] *
                                  table_AS_FA_HG[AS, FA, HG]
print(prob_HT)
 0.0672 0.2528]
```

```
m_AS = table_AS_FA_HG[1, :, :]
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
            for FA in [0, 1]:
                prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                                 table HG HT FG[HG, HT, FG] *
                                 table FA[FA] *
                                 m AS[FA, HG]
print(prob HT)
[ 0.0672 0.2528]
```

# Any ideas to reduce #multiplications?

```
m AS = table AS FA HG[1, :, :]
prob HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
            for FA in [0, 1]:
                prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                                 table HG HT FG[HG, HT, FG] *
                                 table FA[FA] * m AS[FA, HG]
print(prob HT)
[ 0.0672 0.2528]
```

# Loop unrolling

```
m_AS = table_AS_FA_HG[1, :, :]
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
            prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                              table HG HT FG[HG, HT, FG] *
                              table FA[0] * m AS[0, HG] \leftarrow
            prob HT[HT] += (table_FG[FG] * table_HT[HT] *
                              table HG HT FG[HG, HT, FG] *
                              table FA[1] * m AS[1, HG] \leftarrow
print(prob HT)
[ 0.0672 0.2528]
```

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### Rearranging the parentheses

```
m_AS = table_AS_FA_HG[1, :, :]
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
            prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                             table HG HT FG[HG, HT, FG] *
                             (table_FA[∅] * m_AS[∅, HG] + ←
                              table FA[1] * m AS[1, HG] \leftarrow
print(prob HT)
[ 0.0672 0.2528]
```

### Define a message function for FA

```
m AS = table AS FA HG[1, :, :]
def m_FA(HG): return (table_FA[0] * m_AS[0, HG] +
                      table_FA[1] * m_AS[1, HG])
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
            prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                            table HG HT FG[HG, HT, FG] *
                            m FA(HG)
print(prob HT)
[ 0.0672 0.2528]
```

#### Better to precompute m\_FA

```
m_AS = table_AS_FA_HG[1, :, :]
m_FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
            prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                            table HG HT FG[HG, HT, FG] *
                            m FA[HG]
print(prob HT)
[ 0.0672 0.2528]
```

#### FA is removed, then remove HG

```
m_AS = table_AS_FA_HG[1, :, :]
m_FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
prob HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
            prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                            table HG HT FG[HG, HT, FG] *
                            m FA[HG]
print(prob HT)
[ 0.0672 0.2528]
```

# Loop unrolling, rearranging the parentheses

```
m_AS = table_AS_FA_HG[1, :, :]
m FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                        (table_HG_HT_FG[∅, HT, FG] * m_FA[∅] +
                         table HG HT FG[1, HT, FG] * m FA[1]
print(prob_HT)
[ 0.0672 0.2528]
```

### Define a message function for *HG*

```
m_AS = table_AS_FA_HG[1, :, :]
m FA = table FA[0] * m AS[0, :] + table <math>FA[1] * m AS[1, :]
def m_HG(HT, FG): return (table_HG_HT_FG[0, HT, FG] * m_FA[0] +
                           table HG HT FG[1, HT, FG] * m FA[1])
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                        m HG(HT, FG)
print(prob HT)
[ 0.0672 0.2528]
```

# Again, better to precompute m\_HG

```
m_AS = table_AS_FA_HG[1, :, :]
m FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
m HG = (table_HG_HT_FG[∅, :, :] * m_FA[∅] +
        table_HG_HT_FG[1, :, :] * m_FA[1])
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                        m_HG[HT, FG]
print(prob HT)
[ 0.0672 0.2528]
```

### Then FG, directly define the message func

```
m AS = table AS FA HG[1, :, :]
m FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
m_HG = (table_HG_HT_FG[0, :, :] * m_FA[0] +
        table HG HT FG[1, :, :] * m FA[1]
def m_FG(HT): return (table_FG[0] * m_HG[HT, 0] +
                      table_FG[1] * m_HG[HT, 1])
prob_HT = np.zeros(2)
for HT in [0, 1]:
    prob_HT[HT] += m_FG(HT) * table_HT[HT]
print(prob HT)
[ 0.0672 0.2528]
```

#### Finally

```
m AS = table AS FA HG[1, :, :]
m_FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
m_HG = (table_HG_HT_FG[0, :, :] * m_FA[0] +
        table_HG_HT_FG[1, :, :] * m_FA[1])
m_FG = table_FG[0] * m_HG[:, 0] + table_FG[1] * m_HG[:, 1]
prob_HT = m_FG[HT] * table_HT[HT]
print(prob_HT)
[ 0.0672 0.2528]
```

# Finally (how many multiplications?)

```
m_AS = table_AS_FA_HG[1, :, :] 0
m_FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
m HG = (table_HG_HT_FG[∅, :, :] * m_FA[∅] + 4
        table_HG_HT_FG[1, :, :] * m_FA[1]) 4
m_FG = table_FG[∅] * m_HG[:, ∅] + table_FG[1] * m_HG[:, 1]
prob_HT = m_FG[HT] * table_HT[HT]
                      in total 2*2 + 4*2 + 2*2 + 2 = 18
print(prob_HT)
[ 0.0672 0.2528]
```

# Naive way (how many multiplications?)

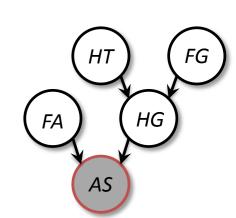
```
AS = 1
prob HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for HG in [0, 1]:
            for FA in [0, 1]:
                prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                                 table HG HT FG[HG, HT, FG] *
                                 table FA[FA] *
                                 table AS FA HG[AS, FA, HG]
                            in total 4 * 16 = 64
print(prob HT)
[ 0.0672 0.2528]
```

### What we have done mathematically?

```
m_AS = table_AS_FA_HG[1, :, :]
                   m_{AS}(FA, HG) = P(AS = 1|FA, HG)
m_FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
                   m_{FA}(HG) = \sum_{TA} P(FA) m_{AS}(FA, HG)
m_HG = (table_HG_HT_FG[0, :, :] * m FA[0] +
         table HG HT FG[1, :, :] * m FA[1]
               m_{HG}(HT,FG) = \sum P(HG|HT,FG)m_{FA}(HG)
m_FG = table_FG[∅] * m_HG[:, ∅] + table_FG[1] * m HG[:, 1]
                  m_{FG}(HT) = \sum_{i} P(FG)m_{HG}(HT, FG)
prob_HT = m_FG[HT] * table_HT[HT]
                    P(AS = 1, HT) = m_{FG}(HT)P(HT)
```

# Nuclear power plant (cont.)

=  $\Pr(HT) \sum_{FG} \Pr(FG) \sum_{HG} \Pr(HG|HT,FG) \sum_{FA} \Pr(FA) \Pr(AS = t|FA,HG)$ eliminate AS: since AS observed, really a no-op



=  $\Pr(HT) \sum_{FG} \Pr(FG) \sum_{HG} \Pr(HG|HT,FG) \sum_{FA} \Pr(FA) m_{AS} (FA,HG)$ eliminate FA: multiplying 1x2 by 2x2

=  $Pr(HT) \sum_{FG} Pr(FG) \sum_{HG} Pr(HG|HT,FG) m_{FA}(HG)$ eliminate HG: multiplying 2x2x2 by 2x1 HT FG
HG O

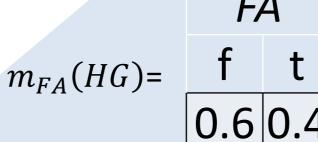
of tables, followed by summing, is actually matrix multiplication

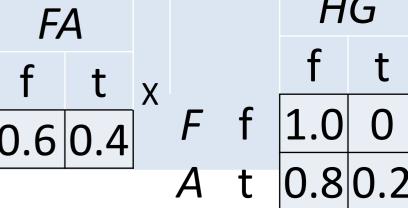
 $= \Pr(HT) \sum_{FG} \Pr(FG) m_{HG}(HT, FG)$ 

eliminate FG: multiplying 1x2 by 2x2

 $= \Pr(HT) \, m_{FG}(HT)$ 







#### But why the order $FA \rightarrow HG \rightarrow FG \rightarrow HT$ ?

```
m_AS[= table_AS_FA_HG[1, :, :] 0
m_FA = table_FA[0] * m_AS[0, :] + table_FA[1] * m_AS[1, :]
m_HG = (table_HG_HT_FG[0, :, :] * m_FA[0] + 4
        table_HG_HT_FG[1, :, :] * m_FA[1]) 4
m_FG = table_FG[0] * m_HG[:, 0] + table_FG[1] * m_HG[:, 1]
prob HT = m_FG[HT] * table_HT[HT]
print(prob HT)
                      in total 2*2 + 4*2 + 2*2 + 2 = 18
 0.0672 0.2528]
```

# Try to eliminate HG after AS

```
HG
m_AS = table_AS_FA_HG[1, :, :]
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for FA in [0, 1]:
            for HG in [0, 1]:
                prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                                 table_HG_HT_FG[HG, HT, FG] *
                                 table FA[FA] *
                                 m AS[FA, HG]
print(prob HT)
[ 0.0672 0.2528]
```

# Try to eliminate HG after AS

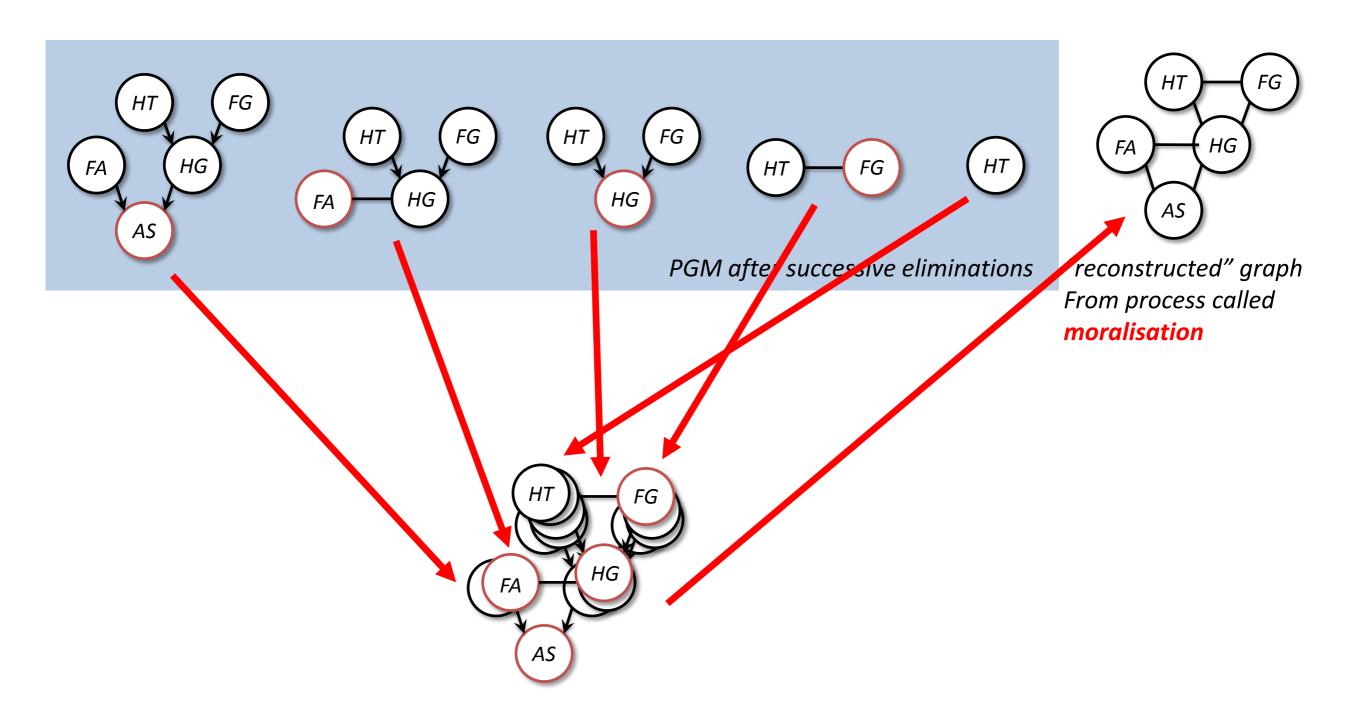
```
m AS = table AS FA HG[1, :, :]
def m_HG(FA, HT, FG): already 8*2 = 16 multiplications
    return (m_AS[FA, 0] * table_HG_HT_FG[0, HT, FG] +
            m AS[FA, 1] * table HG HT FG[1, HT, FG])
                        because HG connected to 3 other nodes
prob_HT = np.zeros(2)
for HT in [0, 1]:
    for FG in [0, 1]:
        for FA in [0, 1]:
            prob_HT[HT] += (table_FG[FG] * table_HT[HT] *
                             table FA[FA] *
                             m HG(FA, HT, FG)
print(prob HT)
[ 0.0672 0.2528]
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```

### A summary for elimination algorithms

An efficient way to marginalize random variables

- ☐ The order of elimination affects the efficiency
  - □ Removing a node with many children and parents results in very large clique (message matrix)
  - Time complexity exponential in the largest clique

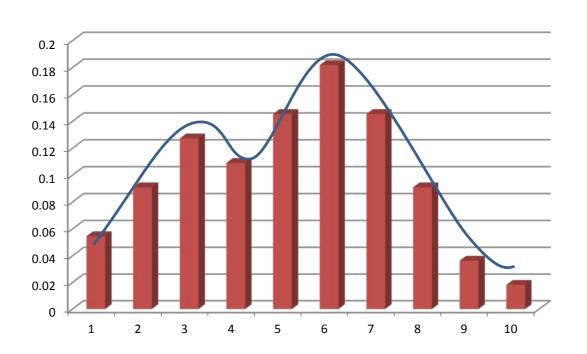
☐ By the way, what is the reconstructed graph?



Put them together -> the reconstructed graph

# Probabilistic inference by simulation

- Exact probabilistic inference can be expensive/impossible
- Can we approximate numerically?
- Idea: sampling methods
  - Cheaply sample from desired distribution
  - Approximate distribution by histogram of samples



## A summary for sampling methods

- ☐ If we get samples, we can
  - use them to calculate expectations (approximately)
  - approximate distributions by histogram of samples

Useful when exact inference is expensive or impossible

- ☐ There are many methods can sample from unnormalized distributions
  - Very useful because normalization is the main challenge for Bayesian inference

### A summary for EM algorithm

- ☐ Designed for MLE when there are latent variables
- $\square$  The joint P(X, Z|w), X observed, Z unobserved, w paras
- $\square$  MLE for w: max<sub>w</sub> log  $P(X|w) = \log \sum_{Z} P(X, Z|w)$
- $\square$  Due to the marginalization for Z, P(X|w) is complicated
  - Gradients are often difficult to calculate
- $\square$  EM can deal with P(X|w) by
  - $\square$  E-step: estimate  $P(\mathbf{Z}|\mathbf{X},\mathbf{w})$
  - $\square$  M-step: MLE for w using P(Z|X, w),  $\max_{w} E_{Z|X,w}[\log P(X, Z|w)]$ 
    - Beneficial because P(X, Z|w) can be factorized
- Sensitive to initialization, may converge to different results

#### Tutor Feedback

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Good luck on your exams!