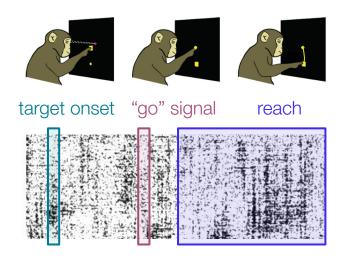
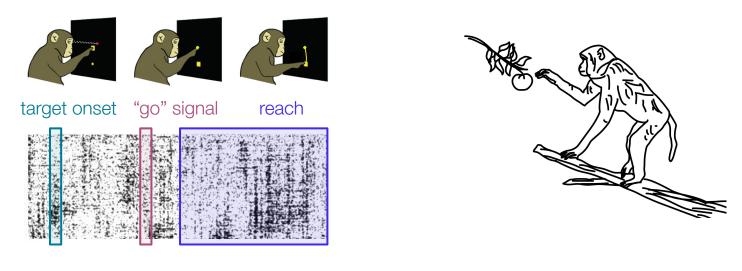
Expectation maximization, mixture models, hidden Markov models

BAMB! '25 Heike Stein

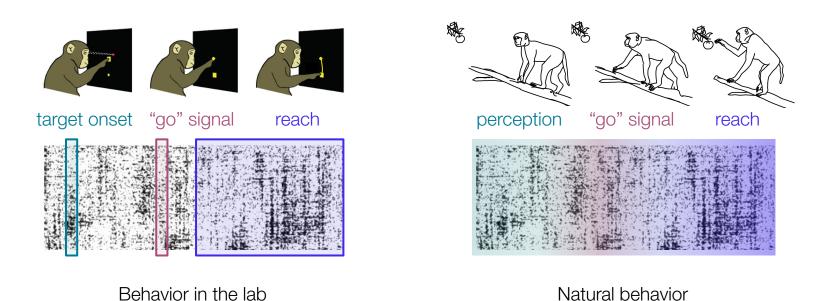


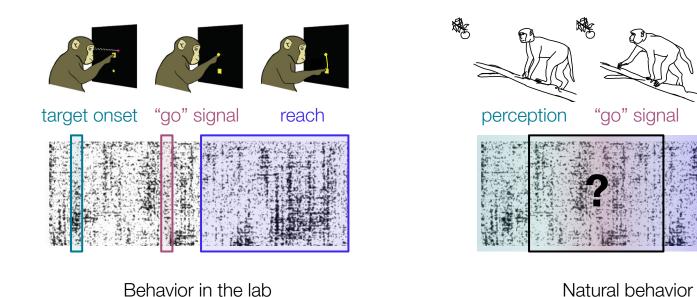
Behavior in the lab

Behavior in the lab



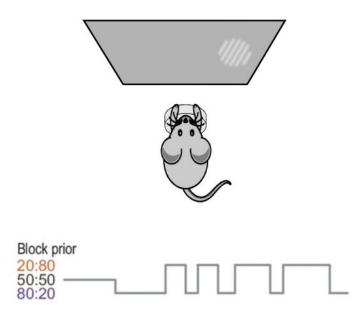
Natural behavior



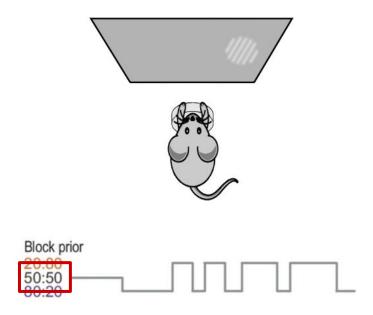


reach

Even in strictly controlled lab-based tasks, we can see unexpected variability in behavior



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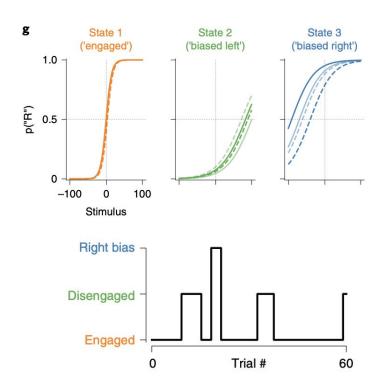
Mice alternate between discrete strategies during perceptual decision-making

Zoe C. Ashwood ^{1,2 ™}, Nicholas A. Roy², Iris R. Stone ², The International Brain Laboratory*, Anne E. Urai ³, Anne K. Churchland ⁴, Alexandre Pouget ⁵ and Jonathan W. Pillow ^{2,6 ™}

Only 50:50 trials!

Even in strictly controlled lab-based tasks, we can see unexpected variability in behavior





Problem: How to deal with uninstructed variability in behavioral patterns?

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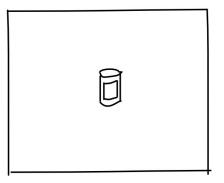
- → We use probabilistic methods (e.g. Bayesian inference) to find latents
- → This will work if the data is explained by a mix of simpler models

What this buys us: We can fit and interpret simple models despite unexpected changes in data patterns

General intro: Probabilistic models

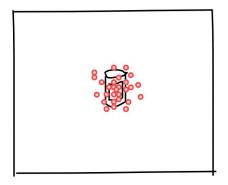
Stochasticity

Behavioral and neural measurements are inherently noisy.



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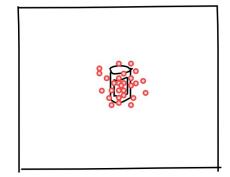


Stochasticity and probabilistic modeling

Behavioral and neural measurements are inherently noisy.

Probabilistic models specify a noise model that

- (1) quantifies variability, and
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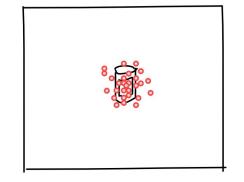


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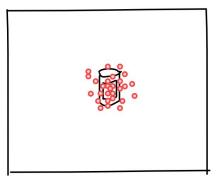


Inference is merely a statistical process of estimating variables or parameters.

It is not assumed to happen in the brain.

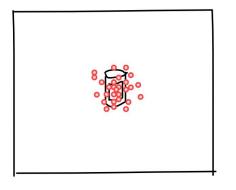
Random variables

A variable X whose value is not deterministic. Its realizations are called observations x



Random variables

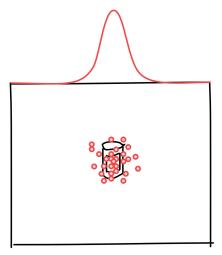
A variable X whose value is not deterministic. Its realizations are called *observations x*



observations $x \in \mathbb{R}^2$ (X is a 2-dimensional, real-valued random variable)

Random variables and distributions

A variable X whose value is not deterministic. Its realizations are called observations x

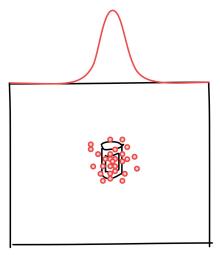


Observations $x \in \mathbb{R}^2$ are distributed according to a Gaussian probability density func.

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

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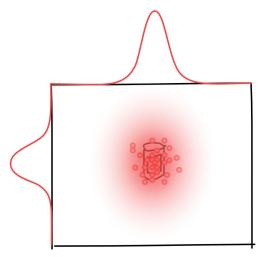


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Observations $x \in \mathbb{R}^2$ are distributed according to a *multivariate Gaussian* pdf

$$f_X(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{d}{2}} \Sigma^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\top} \Sigma^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)$$

Multivariate distributions are joint distributions over random variables

$$\mathbf{X} = (X_1, X_2, ..., X_d)$$
, with a joint PMF or PDF $f_{X_1, X_2, ..., X_d}(X_1, X_2, ..., X_d)$

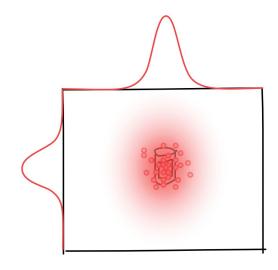
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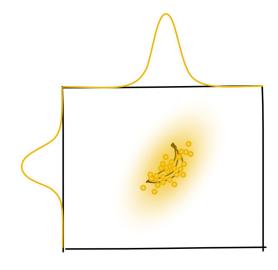
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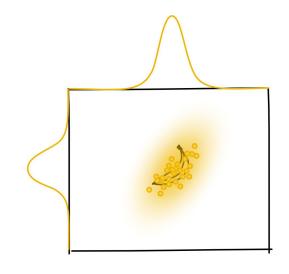
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$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{pmatrix} = \begin{pmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 \end{pmatrix}$$



The likelihood function in probabilistic terms

For different parameter values, how likely is the observed data? $L(\theta \mid \mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_n})$

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- → different parameter values represent different hypotheses about the model
- → the likelihood is the *evidence* for each hypothesis

• the *likelihood* $p(\mathbf{x} \mid \theta)$: evidence for our hypothesis about $|\theta|$

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- the marginal likelihood $p(\mathbf{x}) = \int p(\mathbf{x}|\theta)p(\theta)d\theta$: For any value θ might take, what is the total evidence we have for our model?

Bayesian inference: Combining the likelihood with a prior

In Bayesian statistics, the *likelihood* $p(\mathbf{x} \mid \theta)$ is regarded as *evidence* in favor of a specific parameter set θ . We combine it with our *prior belief (prior distribution)* $p(\theta)$ about how the parameters are distributed to obtain the *posterior distribution* $p(\theta \mid \mathbf{x})$

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Bayes' theorem immediately follows from basic rules of probability, specifically the product rule : $p(\mathbf{B}|\mathbf{A}) = p(\mathbf{A},\mathbf{B}) / p(\mathbf{A})$ $p(\mathbf{A},\mathbf{B}) = p(\mathbf{A}|\mathbf{B}) / p(\mathbf{B})$

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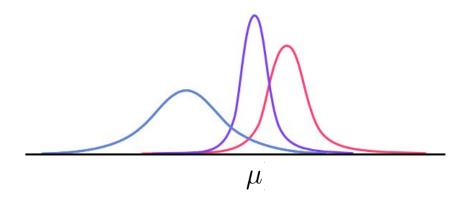
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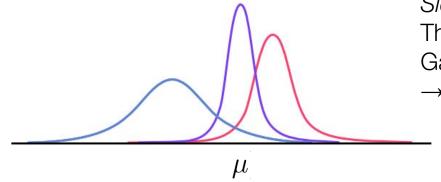
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Side note:

The likelihood is not always Gaussian (e.g. for σ)

→ choose matching, i.e. conjugate priors

Bayesian inference: Combining the likelihood with a prior

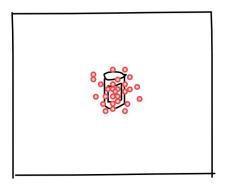
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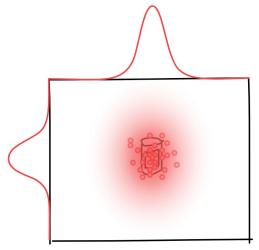
 $p(\mathbf{x}) = \int p(\mathbf{x}|\theta)p(\theta)d\theta$ is a normalization constant to ensure that $p(\theta \mid \mathbf{x})$ integrates to 1. It is called the *marginal likelihood* (sometimes also called *evidence*).

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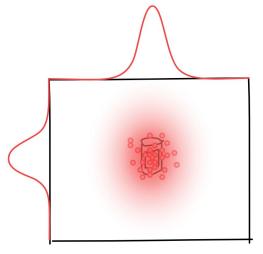


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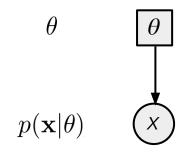


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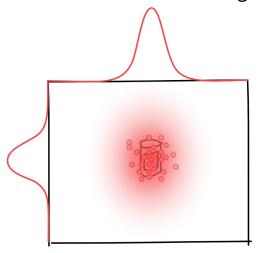
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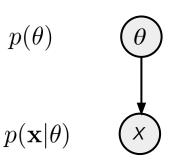
deterministic parameters

observed variables $X = \{X_0, X_1, ..., X_N\}$

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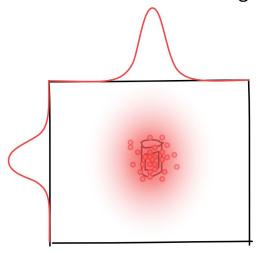
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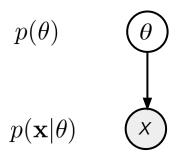
parameters as random variables

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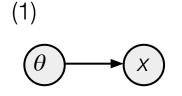
random variables with unknown value (:= *latent variable*)

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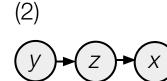
Generative model: Joint distribution of the "complete dataset"

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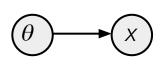
It allows us to write down the *joint distribution* of all variables in our model:



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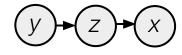
(1)



It allows us to write down the *joint distribution* of all variables in our model:

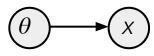
(1)
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$$p(\mathbf{x}, \mathbf{z}, \mathbf{y}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\mathbf{y})p(\mathbf{y})$$



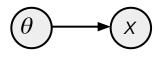
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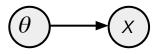
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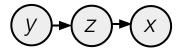


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- sample $\theta = \{\mu, \Sigma\}$ from $p(\theta)$ (or assume fixed values)
- then, with fixed $\theta = \{\mu, \Sigma\}$, sample x from $p(\mathbf{x}|\theta) = \mathcal{N}(\mathbf{x}; \mu, \Sigma)$: $\mathbf{x}_i | \mu, \Sigma \sim \mathcal{N}(\mu, \Sigma)$

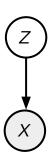
With the generative model, we can sample datasets:

 $p(\mathbf{x}, \mathbf{z}, \mathbf{y}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\mathbf{y})p(\mathbf{y})$ assuming all variables are binary



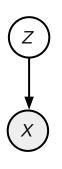
- $\begin{array}{ll} \bullet & \text{sample y: } U \sim \operatorname{Uniform}(0,1) \\ \mathbf{y} = 1_{\{U < p_{\mathbf{v}}\}} \end{array}$
- $\begin{array}{ll} \bullet & \text{sample z: } P(\mathbf{z}=1|\mathbf{y}) = p_{\mathbf{z}|\mathbf{y}}, \quad P(\mathbf{z}=0|\mathbf{y}) = 1 p_{\mathbf{z}|\mathbf{y}} \\ & U \sim \mathrm{Uniform}(0,1) \\ & \mathbf{z} = 1_{\{U \leq p_{\mathbf{z}|\mathbf{y}}\}} \end{array}$
- sample x analogously

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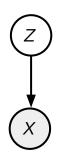
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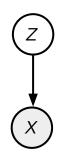
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General recipe:

1) Use Bayesian inference to find a posterior for the latent variable

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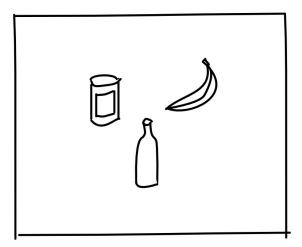
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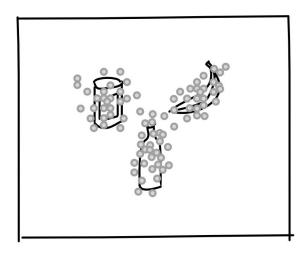
- 1) Use Bayesian inference to find a posterior for the latent variable
- 2) Maximize a likelihood (via ML) that
 - a) considers all possible values of the latent and
 - b) weights them by their probability (the posterior)

Mixture Models and Expectation Maximization

Experiment:

In each trial, subjects have to choose between three objects.



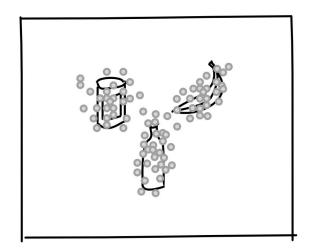




Hypothesis:

For each trial, subjects

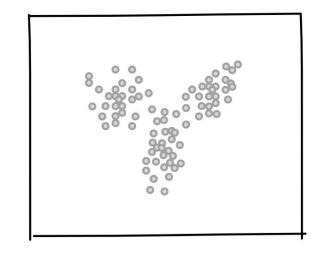
- (1) choose one of three objects, and
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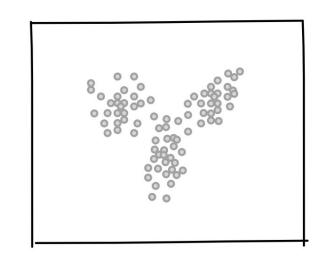


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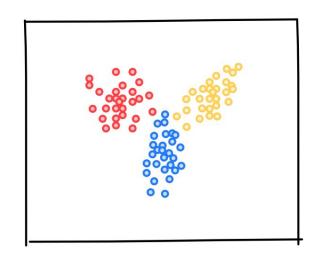
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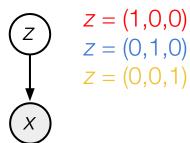
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- (2) make a noisy saccade to the object's center



We assume a categorical, latent variable $\mathbf{z} \in \{0,1\}^{N \times K}$

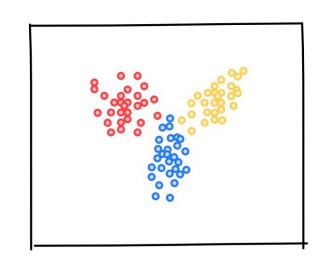


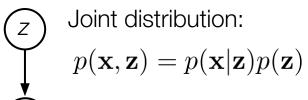
We have only observed saccades $\mathbf{x} \in \mathbb{R}^{N \times D}$

Hypothesis:

For each trial, subjects

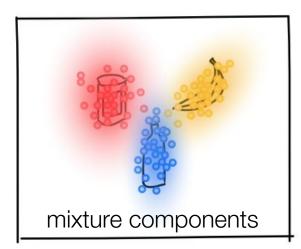
- (1) choose one of three objects, and
- (2) make a noisy saccade to the object's center

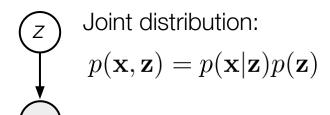




$$p(\mathbf{x}|z_k=1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

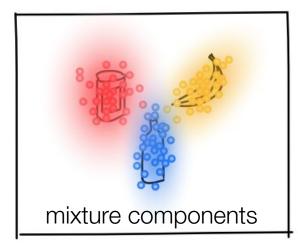
For each class *k*, observations *x* are distributed as a class-specific Gaussian.

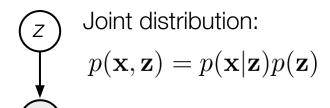




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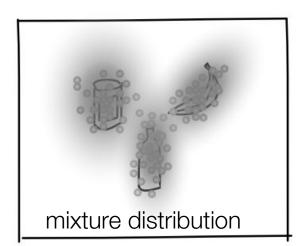


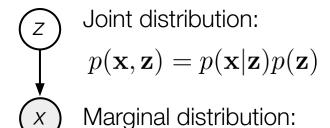


$$p(\mathbf{x}|z_k=1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

For each class *k*, observations **x** are distributed as a class-specific Gaussian.

 $p(z_k = 1) = \pi_k$ The probability of class k(:= mixing coefficient) is its relative frequency.

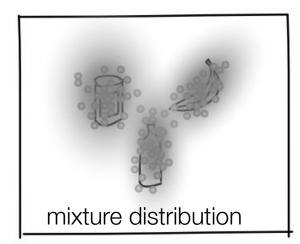


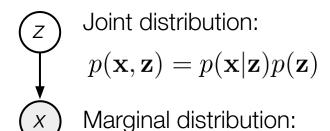


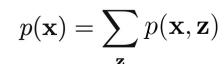
 $p(\mathbf{x})$

$$p(\mathbf{x}|z_k=1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

For each class k, observations \mathbf{x} are distributed as a class-specific Gaussian.

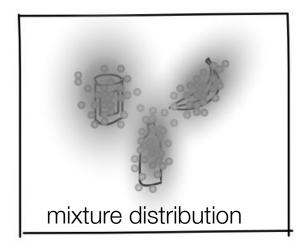


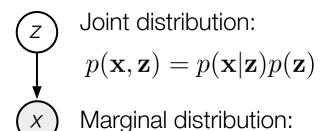




$$p(\mathbf{x}|z_k=1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

For each class *k*, observations **x** are distributed as a class-specific Gaussian.

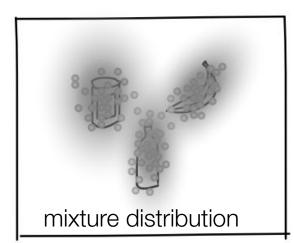


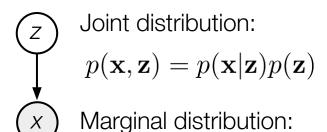


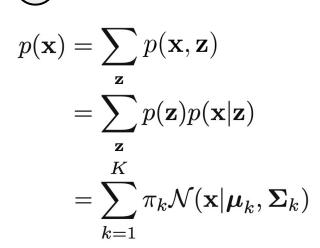
$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z})$$
$$= \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x}|\mathbf{z})$$

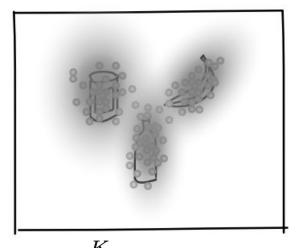
$$p(\mathbf{x}|z_k=1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

For each class *k*, observations **x** are distributed as a class-specific Gaussian.





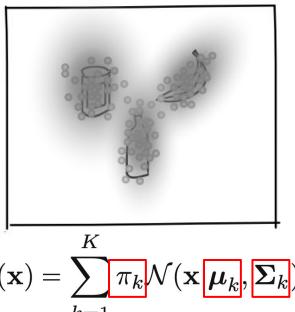




$$p(\mathbf{x}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}|oldsymbol{\mu}_k, oldsymbol{\Sigma}_k)$$

Mixture models

How do we estimate class-specific parameters?

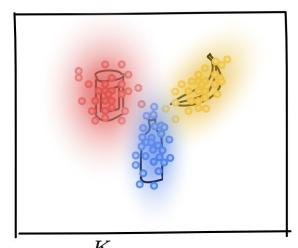


$$p(\mathbf{x}) = \sum_{k=1}^{N} \pi_k \mathcal{N}(\mathbf{x} \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Mixture models

How do we estimate class-specific parameters?

Which data point belongs to which class?

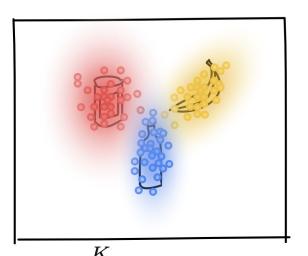


$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Mixture models

How do we estimate class-specific parameters?

Which data point belongs to which class?



Expectation maximization
(EM) is a general algorithm
for parameter estimation in
models of the form

$$p(\mathbf{x}, \mathbf{z}|\theta) = p(\mathbf{x}|\mathbf{z}, \theta)p(\mathbf{z}|\theta)$$

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

EM tackles two problems:

E-Step: Determine which data point belongs to which class

M-Step: Fit class-specific parameters

EM tackles two problems:

E-Step: Determine which data point belongs to which class

→ Inference of the **posterior** over the latent indicator variable **z**

$$p(\mathbf{z}|\mathbf{x}, \theta) = \frac{p(\mathbf{x}|\mathbf{z}, \theta)p(\mathbf{z}|\theta)}{p(\mathbf{x}|\theta)}$$

EM tackles two problems:

E-Step: Determine which data point belongs to which class

→ Inference of the **posterior** over the latent indicator variable **z**

$$p(\mathbf{z}|\mathbf{x}, \theta) = \frac{p(\mathbf{x}|\mathbf{z}, \theta)p(\mathbf{z}|\theta)}{p(\mathbf{x}|\theta)} - \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}|\theta) = \sum_{\mathbf{z}} p(\mathbf{x}|\mathbf{z}, \theta)p(\mathbf{z}|\theta)$$

EM tackles two problems:

E-Step: Determine which data point belongs to which class

→ Inference of the **posterior** over the latent indicator variable **z**

$$p(\mathbf{z}|\mathbf{x}, \theta) = \frac{p(\mathbf{x}|\mathbf{z}, \theta)p(\mathbf{z}|\theta)}{p(\mathbf{x}|\theta)}$$

$$= \frac{\pi_k \mathcal{N}(\mathbf{x}; \mu_k, \Sigma_k)}{\sum_{K} \pi_k \mathcal{N}(\mathbf{x}; \mu_k, \Sigma_k)} \quad \text{for Gaussian mixture models}$$

EM tackles two problems:

E-Step: Determine which data point belongs to which class

→ Inference of the **posterior** over the latent indicator variable **z**

$$p(\mathbf{z}|\mathbf{x}, \theta) = \frac{p(\mathbf{x}|\mathbf{z}, \theta)p(\mathbf{z}|\theta)}{p(\mathbf{x}|\theta)}$$
$$= \frac{\pi_k \mathcal{N}(\mathbf{x}; \mu_k, \Sigma_k)}{\sum_K \pi_k \mathcal{N}(\mathbf{x}; \mu_k, \Sigma_k)}$$

 $= \frac{\pi_k \mathcal{N}(\mathbf{x}; \mu_k, \Sigma_k)}{\sum_K \pi_k \mathcal{N}(\mathbf{x}; \mu_k, \Sigma_k)}$ Then: plug in current parameter estimates, evaluate PDF for each datapoint and each class, normalize

$$\rightarrow$$
 responsibilities $\gamma_{ik} = p(z_{ik} = 1 | x_i, \theta)$

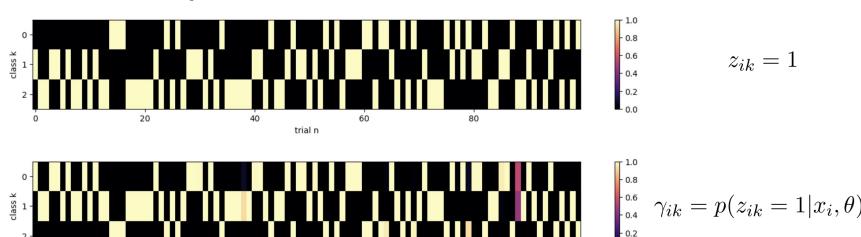
20

EM tackles two problems:

E-Step: Determine which data point belongs to which class

 \rightarrow Inference of the **posterior** over the latent indicator variable z

trial n



EM tackles two problems:

E-Step: Determine which data point belongs to which class

 \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}

M-Step: Fit class-specific parameters

ightarrow Maximize the complete-data log LL $\ln p(\boldsymbol{x}, \boldsymbol{z}|\theta)$

EM tackles two problems:

E-Step: Determine which data point belongs to which class

 \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}

M-Step: Fit class-specific parameters

- \rightarrow Maximize the complete-data log LL $\ln p(\boldsymbol{x}, \boldsymbol{z}|\theta)$
- → Problem: We don't know the value of **z**

- **E-Step:** Determine which data point belongs to which class
 - \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}
- **M-Step:** Fit class-specific parameters
 - \rightarrow Maximize the complete-data log LL $\ln p(\boldsymbol{x}, \boldsymbol{z}|\theta)$
 - → Problem: We don't know the value of **z**
 - **Solution:** Optimize expected value under the posterior distribution of **z**

$$\mathbb{E}_{\mathbf{z}}\left[\ln p(oldsymbol{x},oldsymbol{z}| heta')
ight] = \sum_{oldsymbol{z}} p(oldsymbol{z}|oldsymbol{x}, heta) \ln p(oldsymbol{x},oldsymbol{z}| heta')$$

- **E-Step:** Determine which data point belongs to which class
 - \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}
- **M-Step:** Fit class-specific parameters
 - \rightarrow Maximize the complete-data log LL $\ln p(\boldsymbol{x}, \boldsymbol{z}|\theta)$
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 - → Find parameters that optimize expected complete-data log likelihood

$$\mathbb{E}_{\mathbf{z}}\left[\ln p(\boldsymbol{x},\boldsymbol{z}|\theta')\right] = \sum_{z} p(\boldsymbol{z}|\boldsymbol{x},\theta) \ln p(\boldsymbol{x},\boldsymbol{z}|\theta')$$

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 - \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}
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$$\mathbb{E}_{\mathbf{z}}\left[\ln p(\boldsymbol{x},\boldsymbol{z}|\boldsymbol{\theta}')\right] = \sum_{\boldsymbol{z}} p(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\theta}) \ln p(\boldsymbol{x},\boldsymbol{z}|\boldsymbol{\theta}') \\ p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta}') p(\mathbf{z}|\boldsymbol{\theta}') \\ \text{Gaussian pdf weighted by class-specific mixing coefficient}$$

- **E-Step:** Determine which data point belongs to which class
 - \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}
- **M-Step:** Fit class-specific parameters
 - → Find parameters that optimize expected complete-data log likelihood

$$\mathbb{E}_{\mathbf{z}} \left[\ln p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}') \right] = \sum_{\boldsymbol{z}} p(\boldsymbol{z} | \boldsymbol{x}, \boldsymbol{\theta}) \ln p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}')$$
Posterior probabilities of each class for each class for each datapoint of each datapoint of each class-specific mixing coefficient

EM tackles two problems:

- **E-Step:** Determine which data point belongs to which class
 - \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}
- **M-Step:** Fit class-specific parameters
 - → Find parameters that optimize expected complete-data log likelihood

$$\mathbb{E}_{\mathbf{z}}\left[\ln p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta}')\right] = \sum_{\boldsymbol{x}} p(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{\theta}) \ln p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta}')$$

Class-specific likelihoods Posterior probabilities are summed over all of each class for possible values of **z**

each datapoint

 $p(\mathbf{x}|\mathbf{z}, \theta')p(\mathbf{z}|\theta')$ Gaussian pdf weighted by class-specific mixing coefficient

EM tackles two problems:

E-Step: Determine which data point belongs to which class

 \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}

M-Step: Fit class-specific parameters

→ Find parameters that optimize expected complete-data log likelihood

$$\mathbb{E}_{\mathbf{z}}\left[\ln p(\boldsymbol{x},\boldsymbol{z}|\theta')\right] = \sum_{z} p(\boldsymbol{z}|\boldsymbol{x},\theta) \ln p(\boldsymbol{x},\boldsymbol{z}|\theta')$$

Iterate

EM tackles two problems for any model with observations **x** depending on latents **z**:

E-Step: Determine which data point belongs to which class

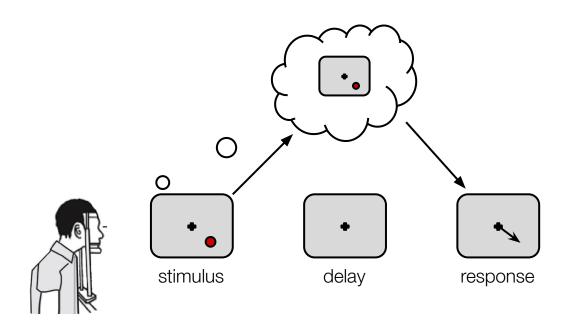
 \rightarrow Inference of the **posterior** $p(\boldsymbol{z}|\boldsymbol{x},\theta)$ over the latent indicator variable \boldsymbol{z}

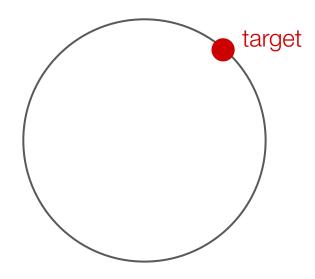
M-Step: Fit class-specific parameters

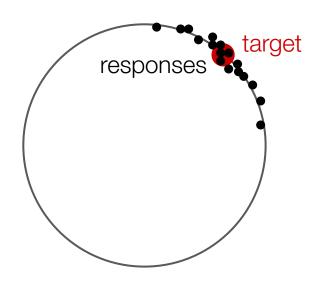
→ Find parameters that optimize expected complete-data log likelihood

$$\mathbb{E}_{\mathbf{z}}\left[\ln p(\boldsymbol{x},\boldsymbol{z}|\theta')\right] = \sum_{z} p(\boldsymbol{z}|\boldsymbol{x},\theta) \ln p(\boldsymbol{x},\boldsymbol{z}|\theta')$$

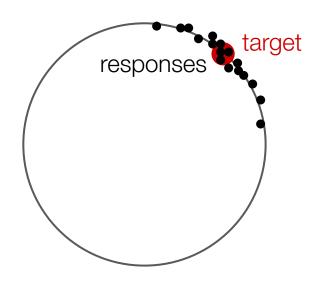
Iterate



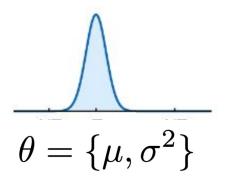


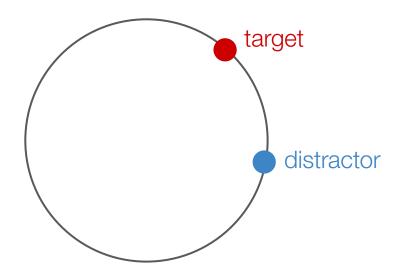


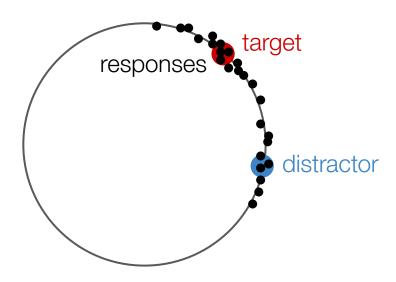
How precise is the working memory representation?

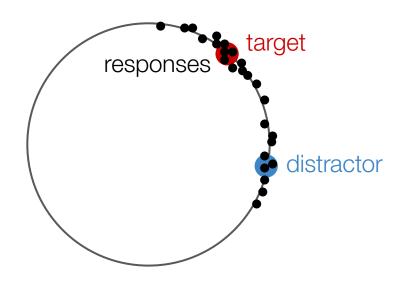


How precise is the working memory representation?

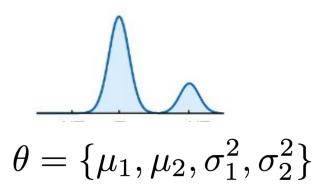








How precise is the working memory representation?

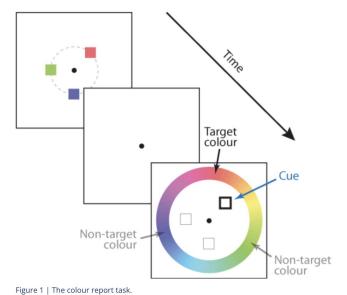


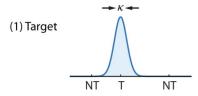
More flexible models are possible! e.g. when target positions change from trial to trial

$$X^{(1)} = X_{\text{saccade}} - X_{\text{target}}$$

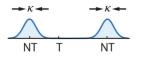
$$X^{(2)} = X_{\text{saccade}} - X_{\text{distractor}}$$

Mixtures of different distributions (e.g. Gaussian, uniform, Student $t... \rightarrow$ last exercise)









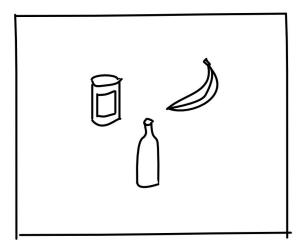
Bays, Catalao & Husain, *J Vis* (2009); Schneegans & Bays, *Cortex* (2016)

(3) Uniform



Experiment:

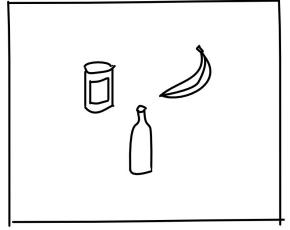
In each trial, subjects have to choose between three objects.

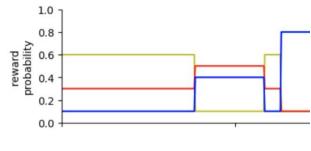


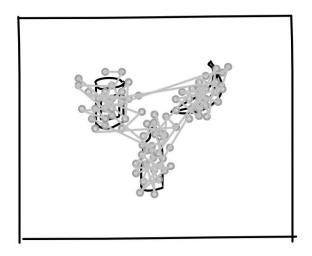
Experiment:

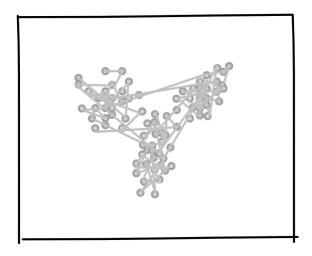
In each trial, subjects have to choose between three objects.

The relative value of objects fluctuates.





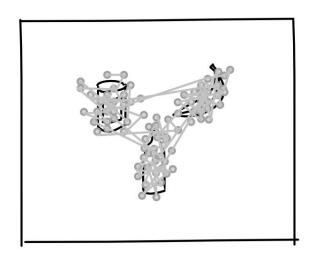




Hypothesis:

For each trial, subjects

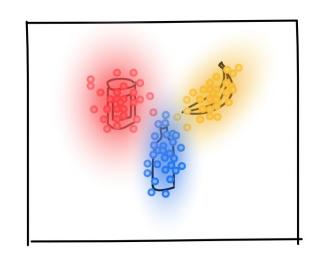
- (1) choose one of three objects
- (2) which object they choose depends on their previous choice
- (3) make a noisy saccade to the object's center



Hypothesis:

For each trial, subjects

- (1) choose one of three objects
- (2) which object they choose depends on their previous choice
- (3) make a noisy saccade to the object's center



latent variable $\mathbf{z} \in \{0,1\}^{N \times K}$

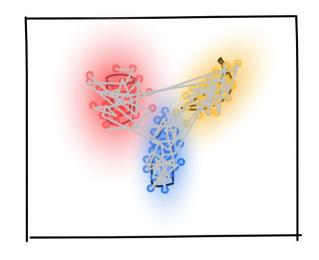
$$\begin{array}{ccc}
z & z = (1,0,0) \\
z & z = (0,1,0) \\
z & z = (0,0,1)
\end{array}$$

observations $\mathbf{x} \in \mathbb{R}^{N \times D}$

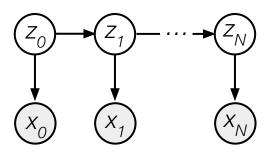
Hypothesis:

For each trial, subjects

- (1) choose one of three objects
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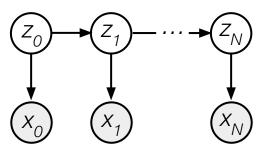
latent variable $\mathbf{z} \in \{0,1\}^{N \times K}$



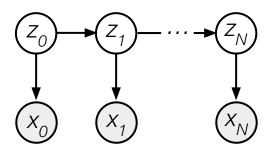
observations $\mathbf{x} \in \mathbb{R}^{N \times D}$

→ temporal dependencies in the latent variable

To capture sequential dependencies in choice behavior, we need an explicit model of transition structure of a latent variable

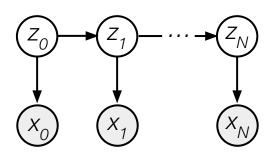


To capture sequential dependencies in choice behavior, we need an explicit model of transition structure of a latent variable



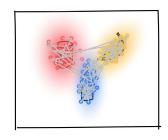
Markov property: $p(\mathbf{z_t}|\mathbf{z_0}, \mathbf{z_1}, ... \mathbf{z_{t-1}}) = p(\mathbf{z_t}|\mathbf{z_{t-1}})$

To capture sequential dependencies in choice behavior, we need an explicit model of transition structure of a latent variable



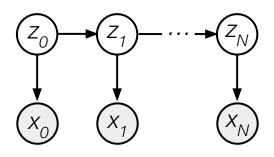
Markov property: $p(\mathbf{z_t}|\mathbf{z_0}, \mathbf{z_1}, ... \mathbf{z_{t-1}}) = p(\mathbf{z_t}|\mathbf{z_{t-1}})$

 \rightarrow We can summarize transition structure in the transition matrix \mathbf{A} , with $A_{jk} \equiv p(z_{nk} = 1 | z_{n-1,j} = 1)$



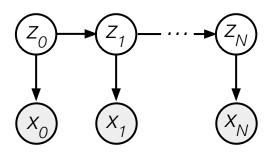


To capture sequential dependencies in choice behavior, we need an explicit model of transition structure of a latent variable



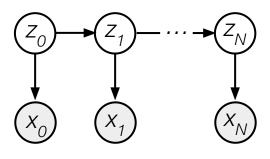
$$p(oldsymbol{x},oldsymbol{z}| heta) = p(oldsymbol{z}_0) \prod_{n=1}^N p(oldsymbol{z}_n|oldsymbol{z}_{n-1}) \prod_{n=0}^N p(oldsymbol{x}_n|oldsymbol{z}_n, heta)$$

To capture sequential dependencies in choice behavior, we need an explicit model of transition structure of a latent variable

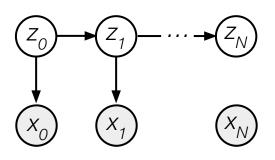


$$p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta}) = p(\boldsymbol{z}_0) \prod_{n=1}^{N} p(\boldsymbol{z}_n|\boldsymbol{z}_{n-1}) \prod_{n=0}^{N} p(\boldsymbol{x}_n|\boldsymbol{z}_n, \boldsymbol{\theta})$$
 initial transition likelihoods state matrix

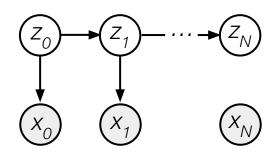
To capture sequential dependencies in choice behavior, we need an explicit model of transition structure of a latent variable



$$p(m{x},m{z}| heta) = p(m{z}_0) \prod_{n=1}^N p(m{z}_n|m{z}_{n-1}) \prod_{n=0}^N p(m{x}_n|m{z}_n, heta)$$
 initial transition likelihoods state matrix π A $\mathcal{N}(m{x}_n;\mu_k,\Sigma_k)$



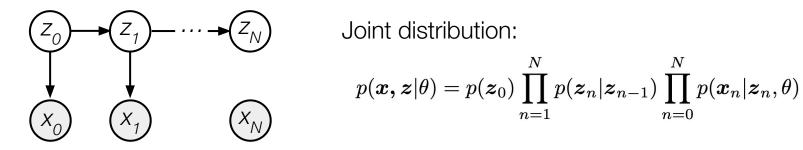
$$p(oldsymbol{x},oldsymbol{z}| heta) = p(oldsymbol{z}_0) \prod_{n=1}^N p(oldsymbol{z}_n|oldsymbol{z}_{n-1}) \prod_{n=0}^N p(oldsymbol{x}_n|oldsymbol{z}_n, heta)$$



Joint distribution:

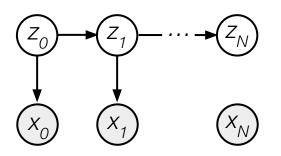
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We want to infer the latent states \mathbf{z} , and estimate parameters $\theta = \{\pi, \mathbf{A}, \mu, \Sigma\}$



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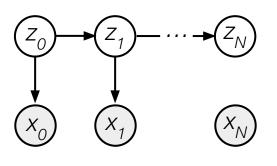
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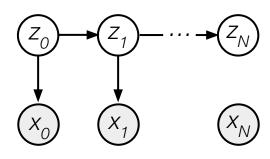
We want to infer the latent states ${m z}$, and estimate parameters ${m heta} = \{{m \pi}, {m A}, {m \mu}, {m \Sigma}\}$

E-Step: infer posteriors, and calculate initial and state transition probabilitie π, A

M-Step: update parameters μ , Σ based on complete-data likelihood

$$ightarrow$$
 easy: optimize expected complete data log LL $\mathbb{E}_{\mathbf{z}}\left[\ln p(\boldsymbol{x}, \boldsymbol{z}|\theta')\right]$

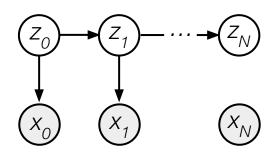
$$=\sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}, \theta) \ln p(\mathbf{x}, \mathbf{z}|\theta')$$



Joint distribution:

$$p(\boldsymbol{x}, \boldsymbol{z} | \theta) = p(\boldsymbol{z}_0) \prod_{n=1}^N p(\boldsymbol{z}_n | \boldsymbol{z}_{n-1}) \prod_{n=0}^N p(\boldsymbol{x}_n | \boldsymbol{z}_n, \theta)$$

E-Step: infer posteriors



Joint distribution:

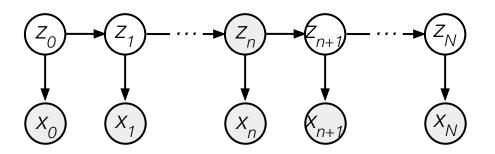
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E-Step: infer posteriors

 \rightarrow In HMMs, there are two posteriors over z:

$$p(\boldsymbol{z}_n|\boldsymbol{x}, heta) \ p(\boldsymbol{z}_n, \boldsymbol{z}_{n-1}|\boldsymbol{x}, heta)$$

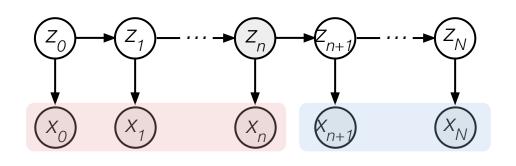
probability of each latent state value, given observations probability of observing a pair of subsequent states, – " –



E-Step: infer posteriors

$$o$$
 again, we start from Bayes theorem $p(\boldsymbol{z}_n|\boldsymbol{x}_{0:N},\theta) = \frac{p(\boldsymbol{x}_{0:N}|\boldsymbol{z}_n,\theta)p(\boldsymbol{z}_n)}{p(\boldsymbol{x}_{0:N})}$

(and equivalent for $p(\boldsymbol{z}_n, \boldsymbol{z}_{n-1} | \boldsymbol{x}, \theta)$)

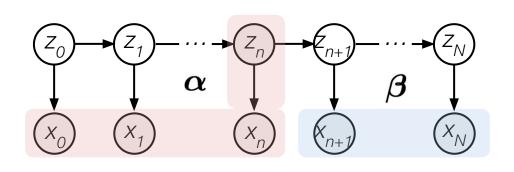


For a given state \mathbf{z}_n for sample n, we can split the likelihood in two terms:

$$p(\boldsymbol{x}_{0:n}|\boldsymbol{z}_n, \theta)$$
, $p(\boldsymbol{x}_{n+1:N}|\boldsymbol{z}_n, \theta)$

E-Step: infer posteriors

ightarrow again, we start from Bayes theorem $p(\boldsymbol{z}_n|\boldsymbol{x}_{0:N},\theta) = \frac{p(\boldsymbol{x}_{0:N}|\boldsymbol{z}_n,\theta)p(\boldsymbol{z}_n)}{p(\boldsymbol{x}_{0:N})}$



We include $p(\boldsymbol{z}_n)$:

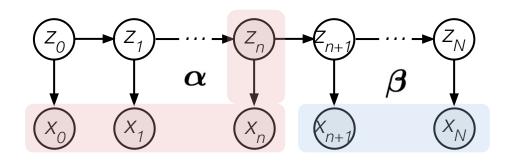
$$egin{aligned} oldsymbol{p}(oldsymbol{x}_{0:n},oldsymbol{z}_n| heta) \ oldsymbol{lpha} oldsymbol{eta} \end{aligned}$$

E-Step: infer posteriors

$$ightarrow$$
 again, we start from Bayes theorem $p(m{z}_n|m{x}_{0:N}, heta) = rac{p(m{x}_{0:N}|m{z}_n, heta)p(m{z}_n)}{p(m{x}_{0:N})}$

→ Then the posterior becomes

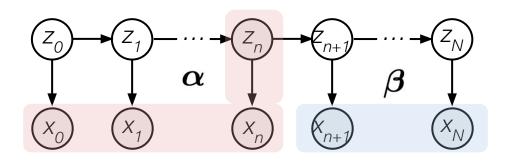
$$p(oldsymbol{z}_n|oldsymbol{x}_{0:N}, heta) = rac{oldsymbol{lpha}(oldsymbol{z}_n)oldsymbol{eta}(oldsymbol{z}_n)}{p(oldsymbol{x}_{0:N})}$$



E-Step: infer posteriors

→ Good news:

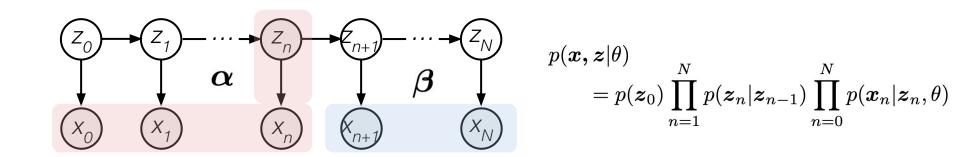
1. There is an efficient algorithm for calculating lpha and eta (the Baum-Welch / forward-backward algorithm)



E-Step: infer posteriors

→ Good news:

- 1. There is an efficient algorithm for calculating α and β (the Baum-Welch / forward-backward algorithm)
- 2. Both posteriors ($p(\boldsymbol{z}_n|\boldsymbol{x},\theta)$ and $p(\boldsymbol{z}_n,\boldsymbol{z}_{n-1}|\boldsymbol{x},\theta)$) can be calculated from $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$



E-Step:

Baum-Welch algorithm to infer posteriors $p(\boldsymbol{z}_n|\boldsymbol{x},\theta)$ and $p(\boldsymbol{z}_n,\boldsymbol{z}_{n-1}|\boldsymbol{x},\theta)$ \rightarrow this also gives us probabilities $\boldsymbol{\pi},\boldsymbol{A}$

M-Step:

update parameters μ, Σ based on complete-data log likelihood $\mathbb{E}_{\mathbf{z}} \left[\ln p(\boldsymbol{x}, \boldsymbol{z} | \theta') \right]$

Gaussian emission models:
$$p(\boldsymbol{x}|z_k=1,\theta_k)=\mathcal{N}(\boldsymbol{x}|\mu_k,\Sigma_k)$$

Other (including more complex) emission models are possible:

- Student-t, etc... (continuous observations x)
- Categorical emissions, Poisson emissions etc (discrete observations x)

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- Autoregressive models: $p(\boldsymbol{x}_n|z_k=1,\theta_k)=\mathcal{N}(\boldsymbol{x}_n|\boldsymbol{A}_k\boldsymbol{x}_{n-1}+d_k,\Sigma_k)$

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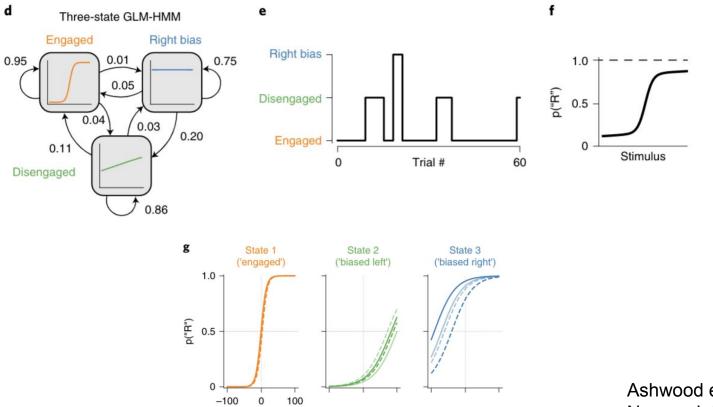
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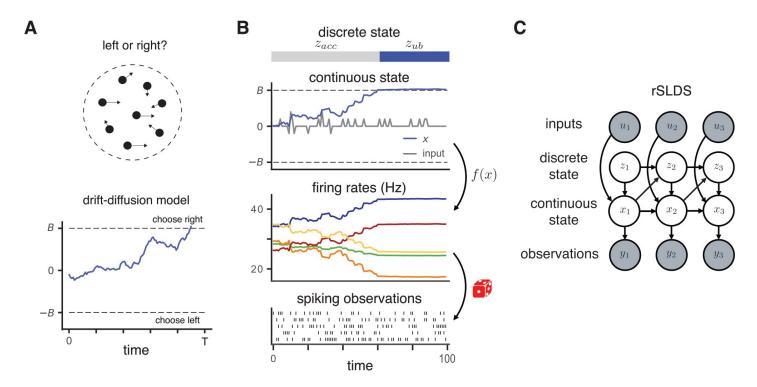
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- Combine them, you get switching drift diffusion models
- Switching factor analysis (if you include an extra set of continuous latents that depend on the state)

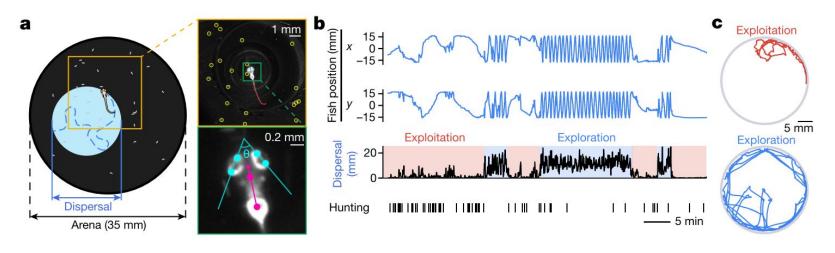


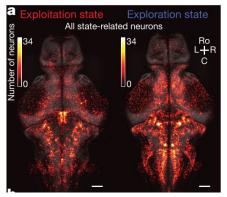
Stimulus

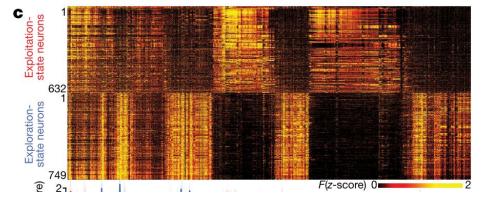
Ashwood et al., Nat Neurosci, 2022



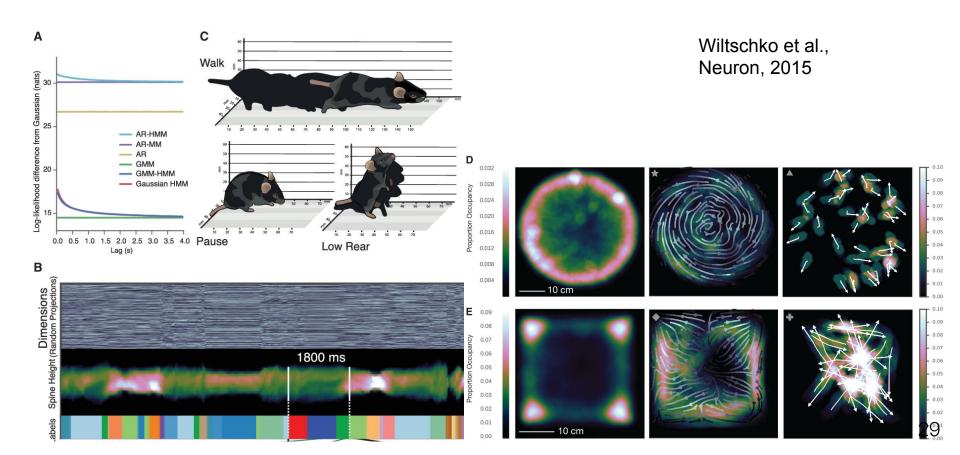
Zoltowski et al., ICML, 2020



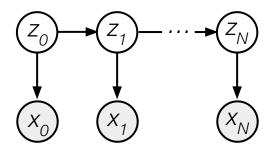




Marques et al., Nature, 2019

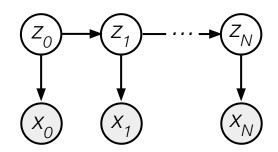


The generative model is the same as for the HMM



$$p(\mathbf{x}, \mathbf{z}|\theta) = p(\mathbf{z}_0|\theta) \prod_{n=1}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1}, \theta) p(\mathbf{x}_n|\mathbf{z}_n, \theta)$$

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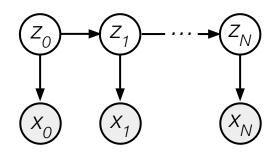
Joint distribution:

$$p(\mathbf{x}, \mathbf{z}|\theta) = p(\mathbf{z}_0|\theta) \prod_{n=1}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1}, \theta) p(\mathbf{x}_n|\mathbf{z}_n, \theta)$$

But now the latent z is continuous-valued, with transition dynamics determined by

$$p(\mathbf{z}_n|\mathbf{z}_{n-1},\theta) = \mathcal{N}(\mathbf{z}_n;\mathbf{A}\mathbf{z}_{n-1},\mathbf{Q})$$

The generative model is the same as for the HMM



Joint distribution:

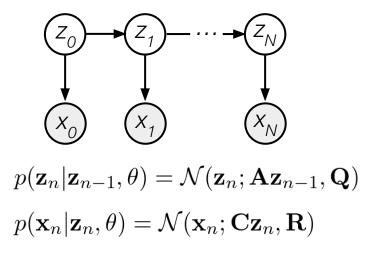
$$p(\mathbf{x}, \mathbf{z}|\theta) = p(\mathbf{z}_0|\theta) \prod_{n=1}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1}, \theta) p(\mathbf{x}_n|\mathbf{z}_n, \theta)$$

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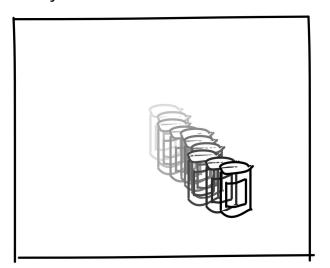
$$p(\mathbf{z}_n|\mathbf{z}_{n-1},\theta) = \mathcal{N}(\mathbf{z}_n;\mathbf{A}\mathbf{z}_{n-1},\mathbf{Q})$$

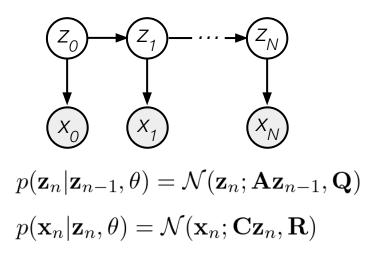
Observations depend linearly on the state **z**

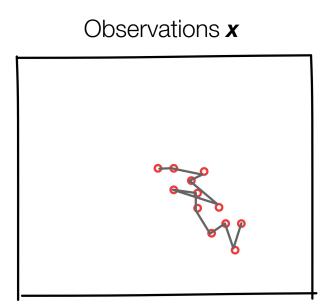
$$p(\mathbf{x}_n|\mathbf{z}_n,\theta) = \mathcal{N}(\mathbf{x}_n; \mathbf{C}\mathbf{z}_n, \mathbf{R})$$

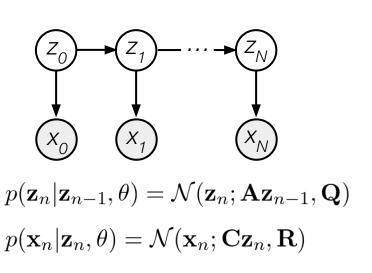


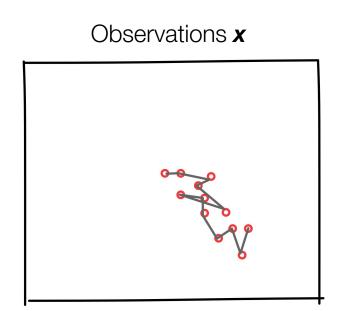
Dynamics of the latent z











 \rightarrow Inference: Posterior for state z and parameters A, C, Q, R

Inference: Posterior for state \mathbf{z} and parameters in $p(\mathbf{z}_n|\mathbf{z}_{n-1},\theta) = \mathcal{N}(\mathbf{z}_n;\mathbf{A}\mathbf{z}_{n-1},\mathbf{Q})$ $p(\mathbf{x}_n|\mathbf{z}_n,\theta) = \mathcal{N}(\mathbf{x}_n;\mathbf{C}\mathbf{z}_n,\mathbf{R})$

E-Step:

Forward-backward algorithm to obtain smoothing posterior $p(\mathbf{z}_n|\mathbf{x}_{0:N},\theta)$ and state transition posterior $p(\mathbf{z}_n|\mathbf{z}_{n-1},\mathbf{x}_{1:N},\theta)$

M-Step:

update parameters **A**, **Q**, **C**, **R** based on complete-data log likelihood $\mathbb{E}_{\mathbf{z}}\left[\ln p(\boldsymbol{x}, \boldsymbol{z} | \theta')\right]$

Further reading & materials

- Textbook on probabilistic statistics and machine learning:
 Christopher Bishop's "Pattern Recognition and Machine Learning" (2006)
- Library for HMMs with all types of emission models:
 Scott Linderman's SSM library https://github.com/lindermanlab/ssm