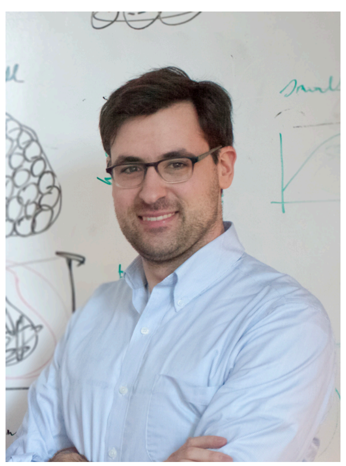
Composing graphical models with neural networks like chocolate and peanut butter

https://youtu.be/O7oD_oX-Gio


David Duvenaud


Alex Wiltchko


Matthew D. Hoffman


Dustin Tran


Scott Linderman


Sandeep Robert Datta


Ryan P. Adams

Google AI

Matthew J Johnson (mattjj@google.com)

July 22 2019 @ UAI 2019

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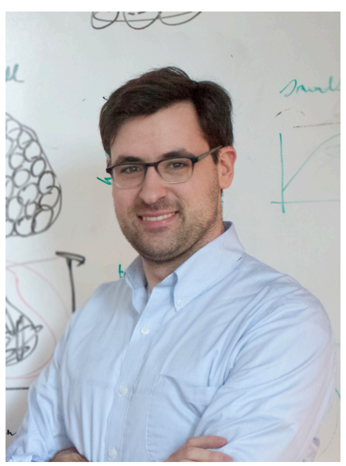
or

Graphical models and exponential families in the age of differentiable programming



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Non-goals

1. Cover the recent literature on PGMs + DNNs
2. Unpack all the technical details

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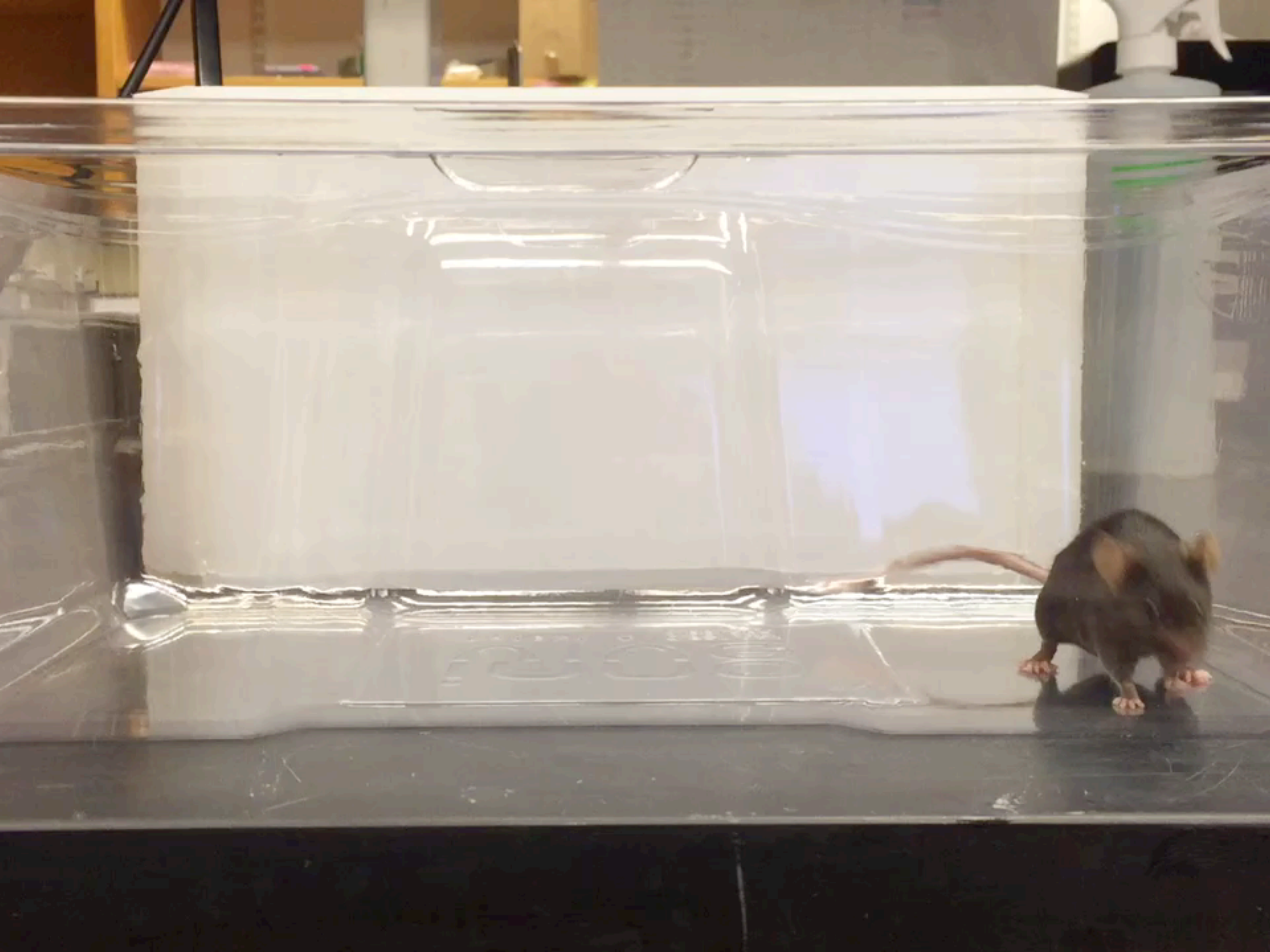

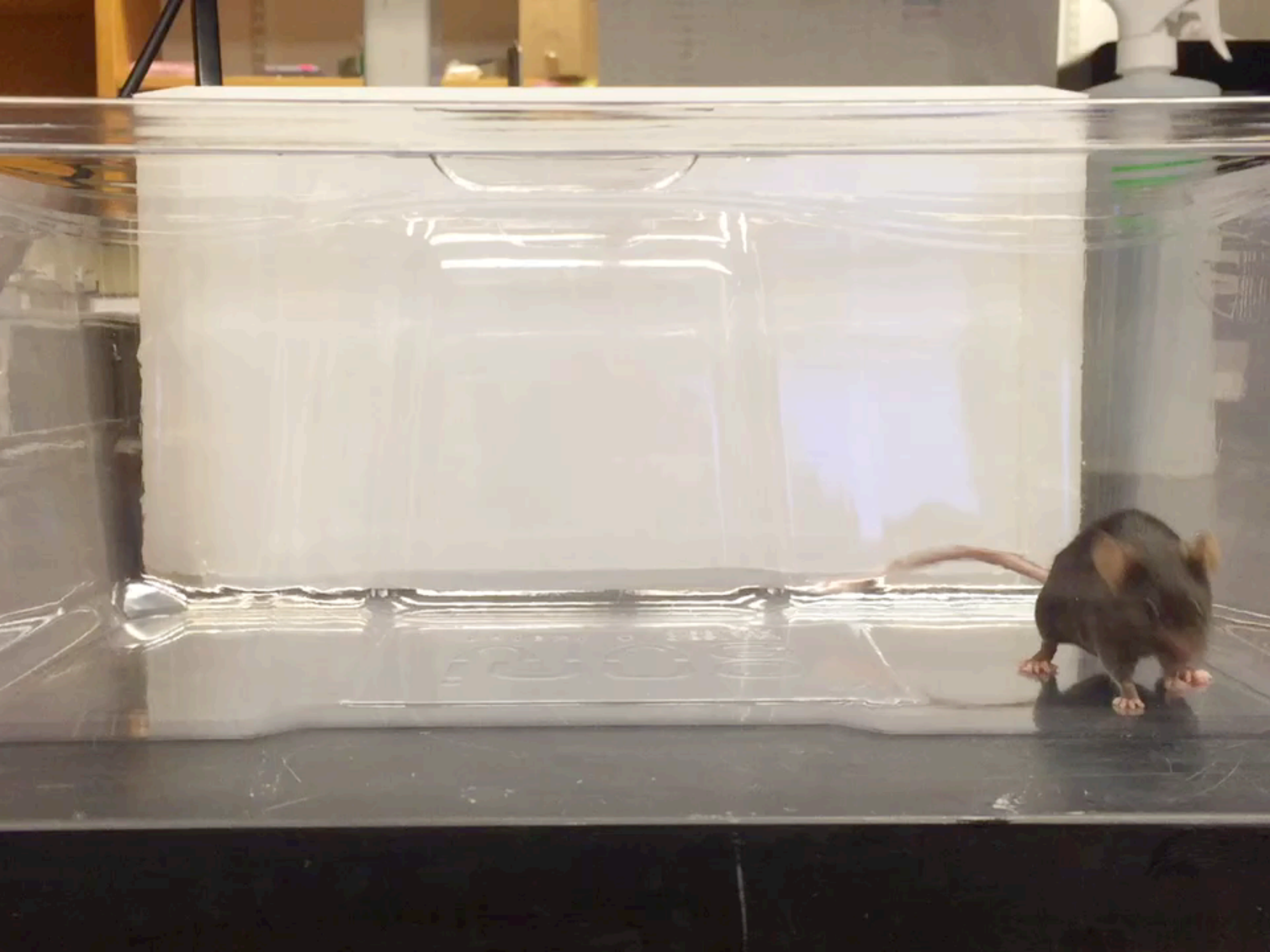

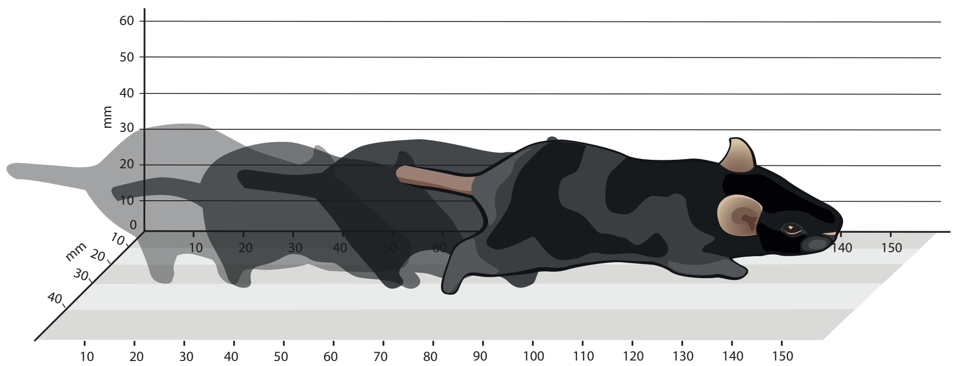

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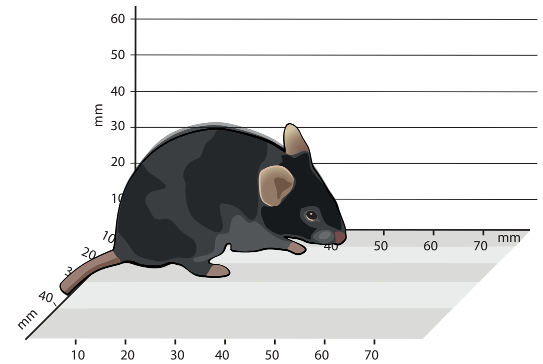

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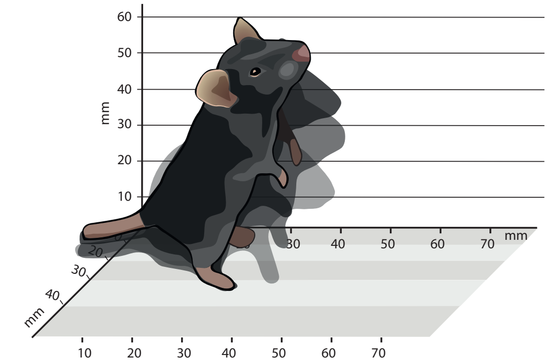

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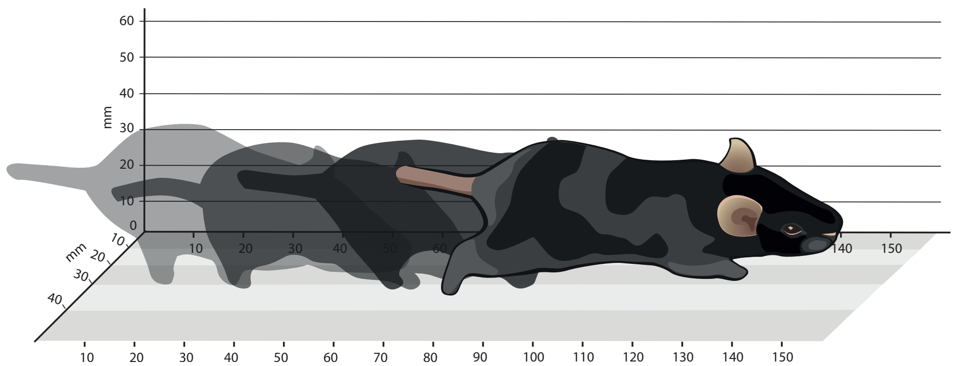

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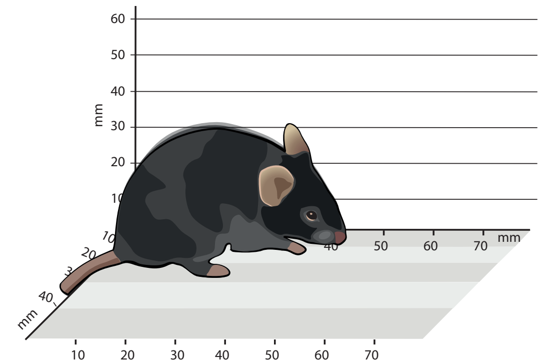

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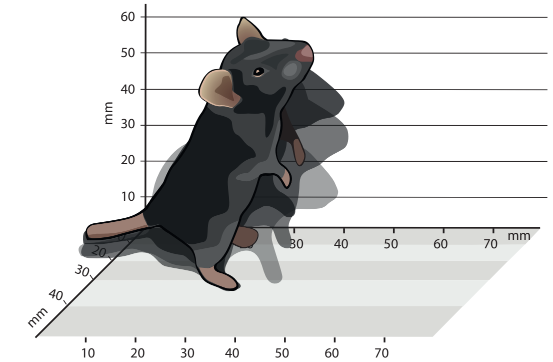

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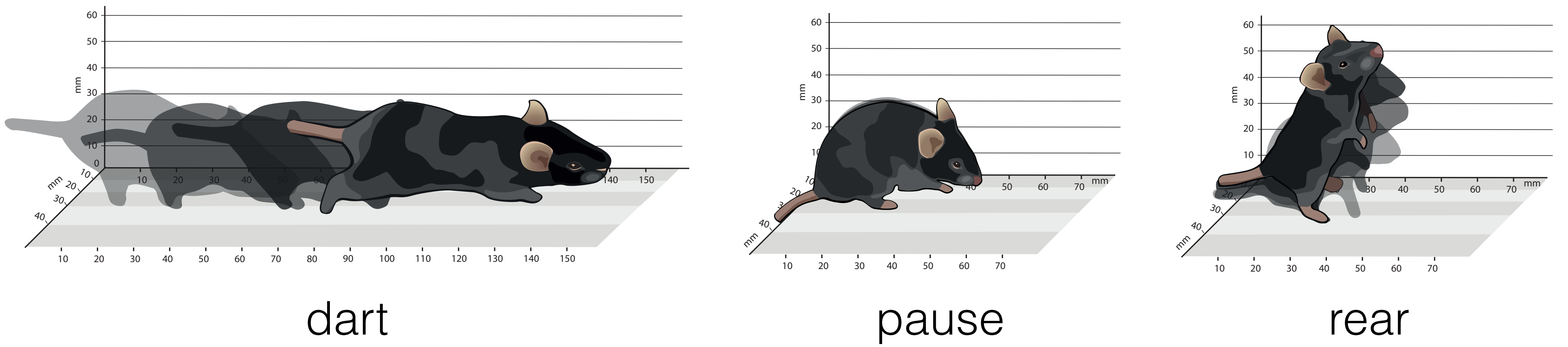
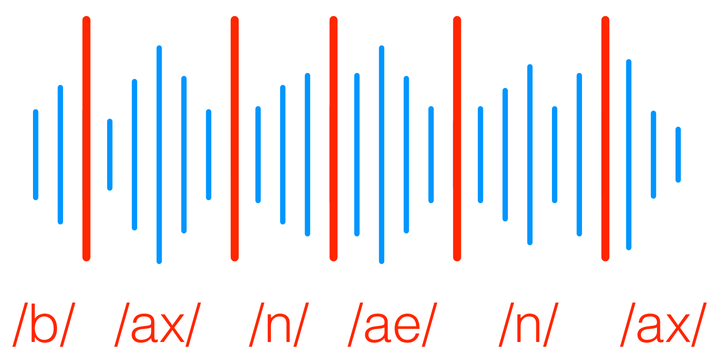
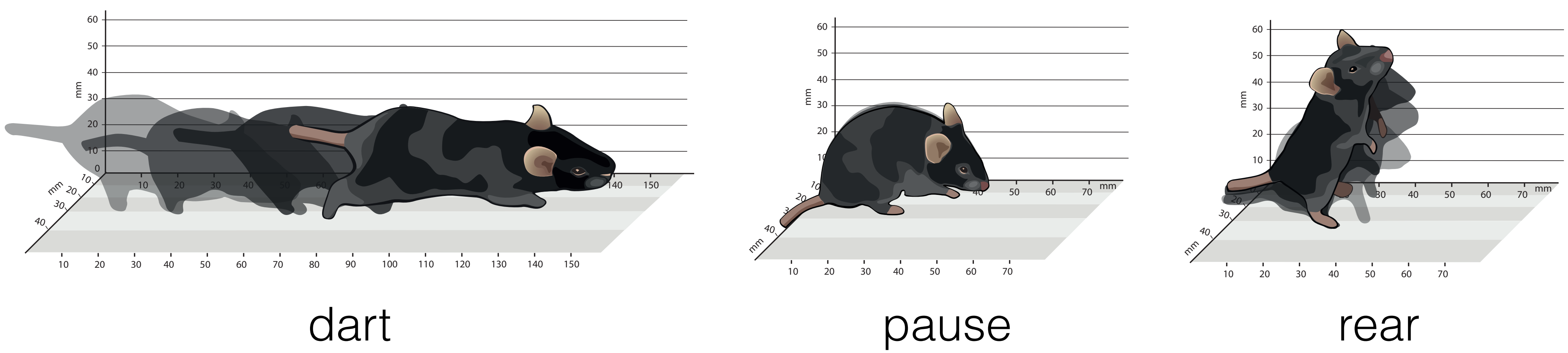
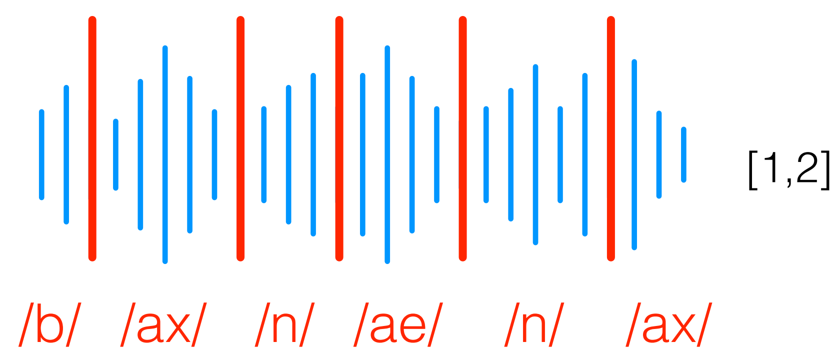


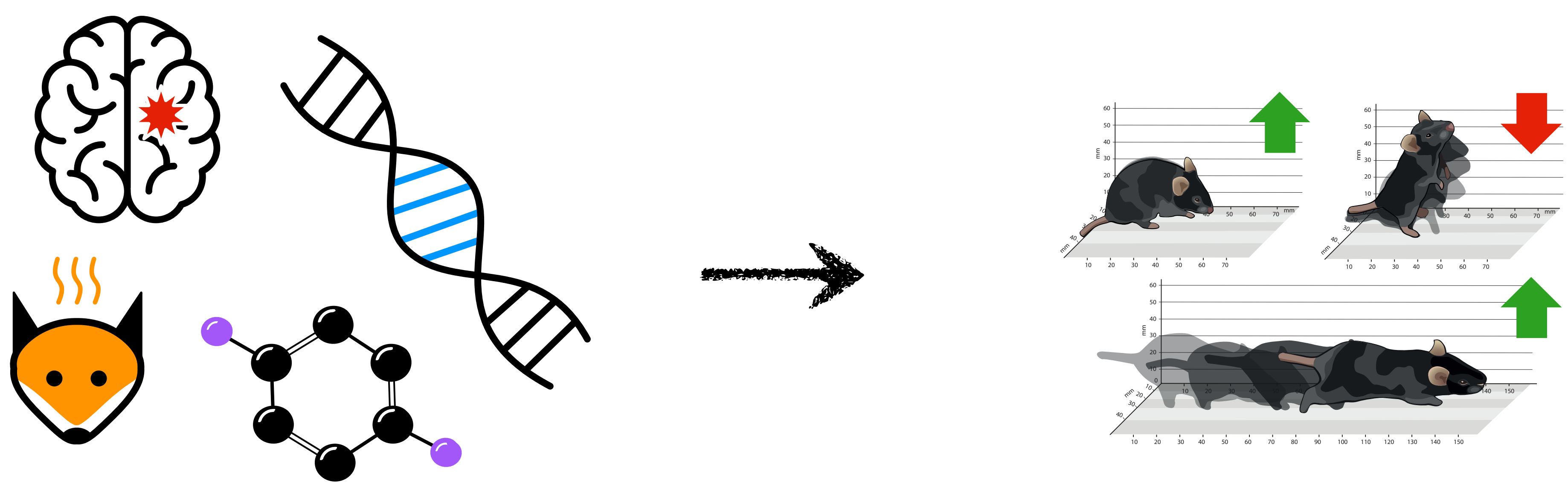


[1,2]

[1] Lee and Glass. A Nonparametric Bayesian Approach to Acoustic Model Discovery. ACL 2012.
[2] Lee. Discovering Linguistic Structures in Speech: Models and Applications. MIT Ph.D. Thesis 2014.







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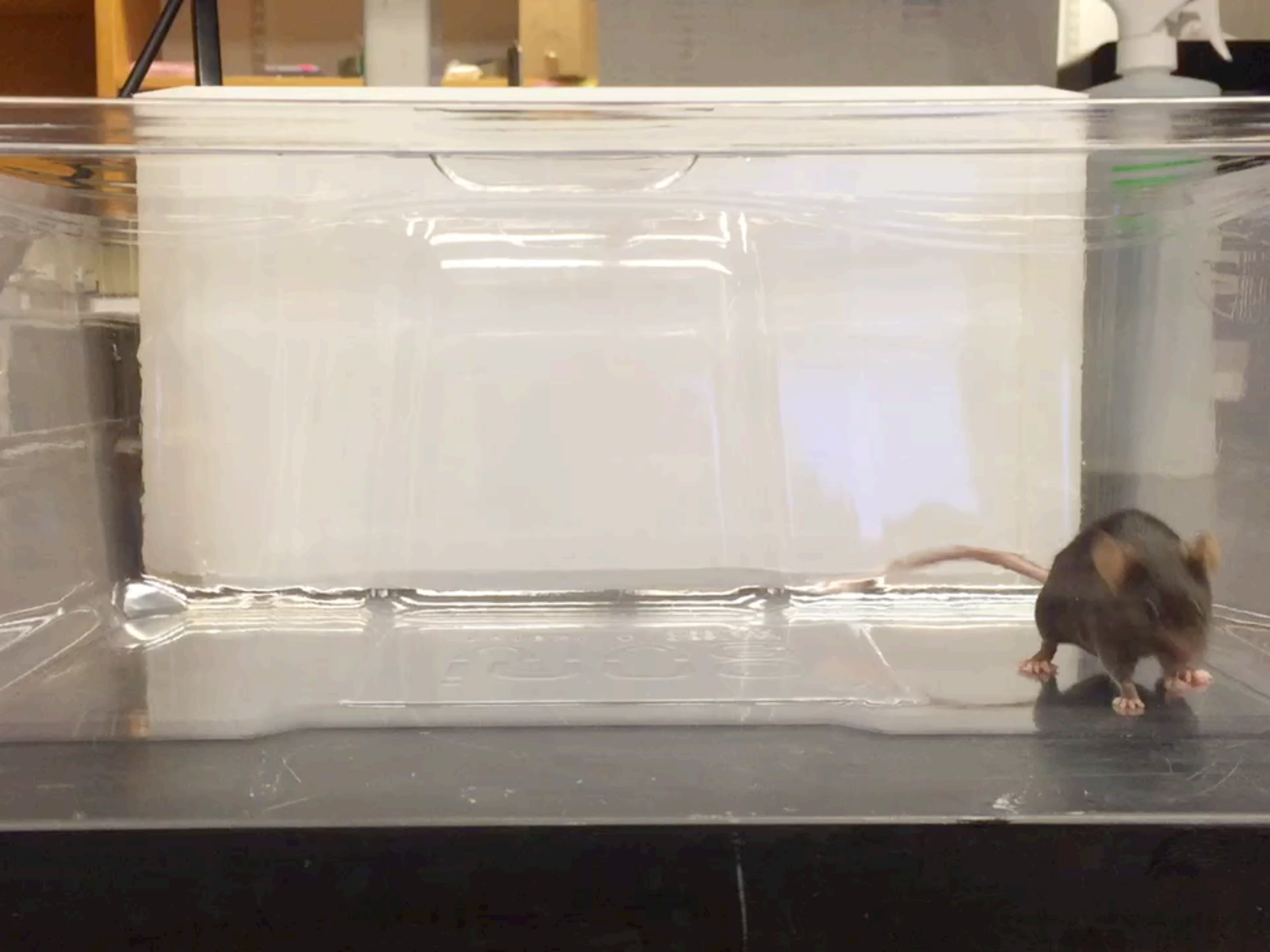

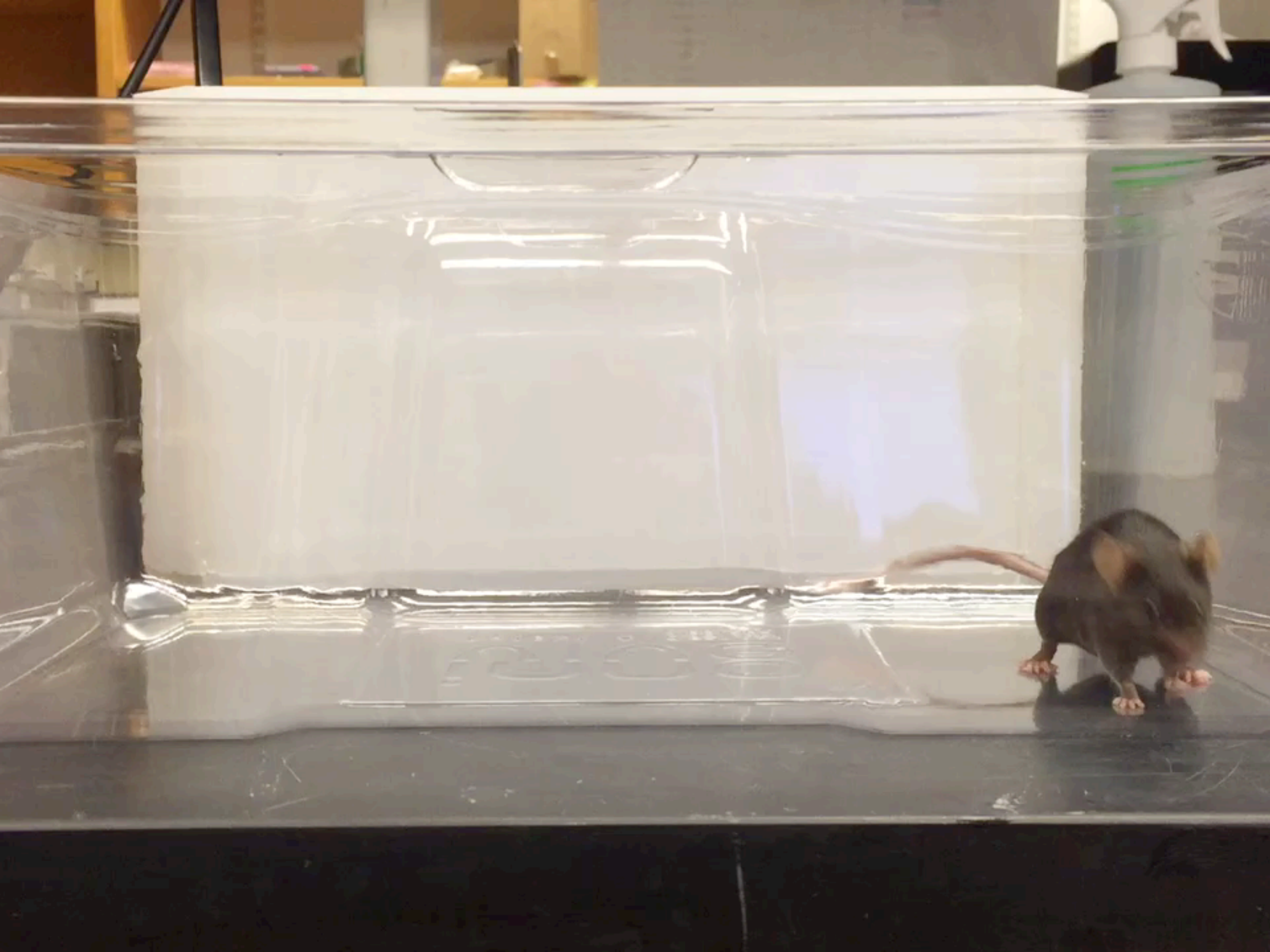

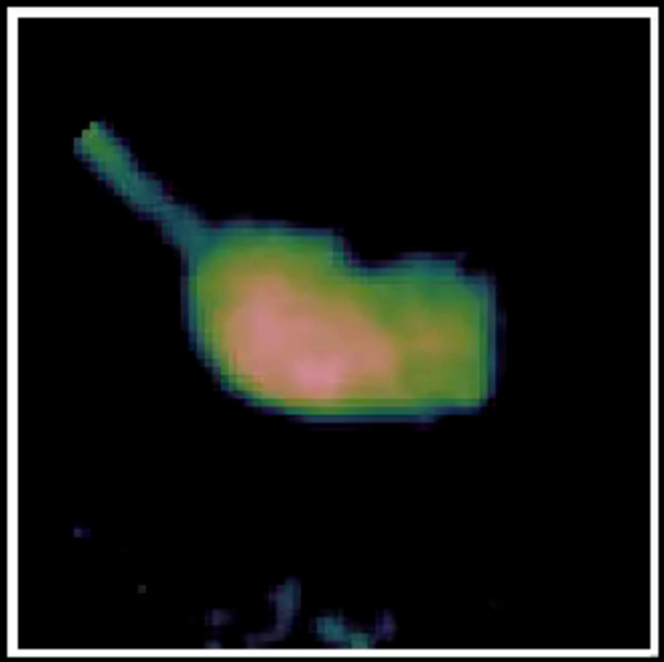

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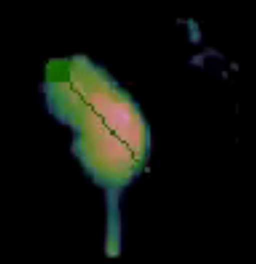

Alexander Wiltschko, **Matthew Johnson**, et al., Neuron 2015.

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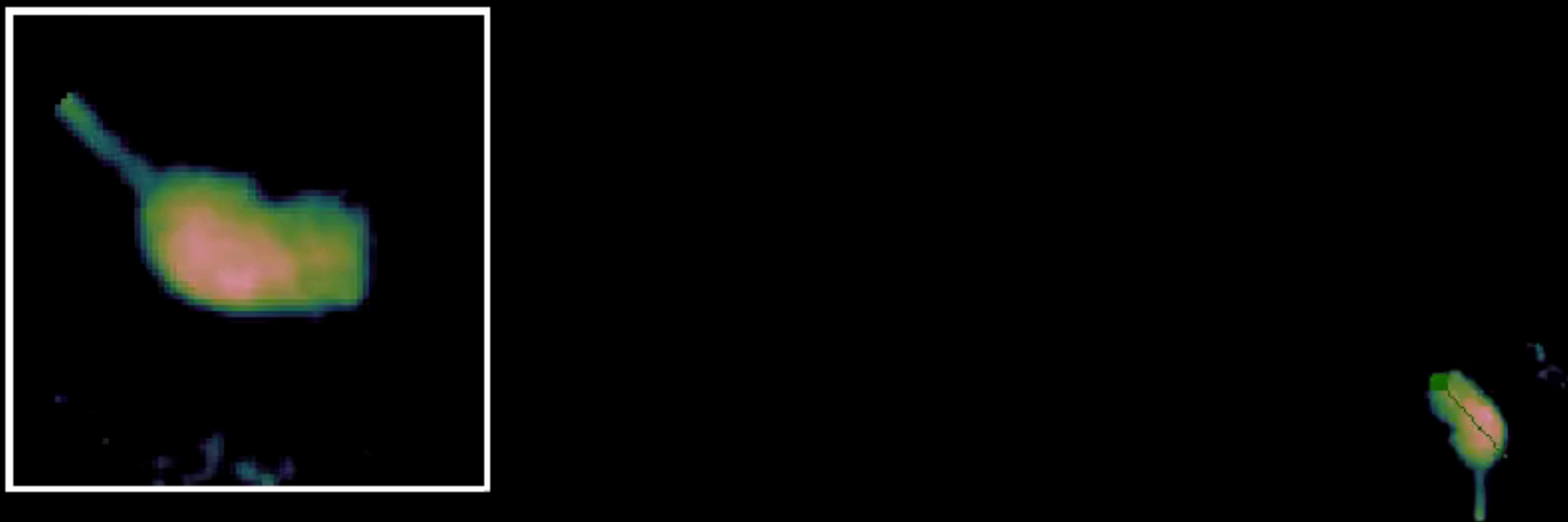

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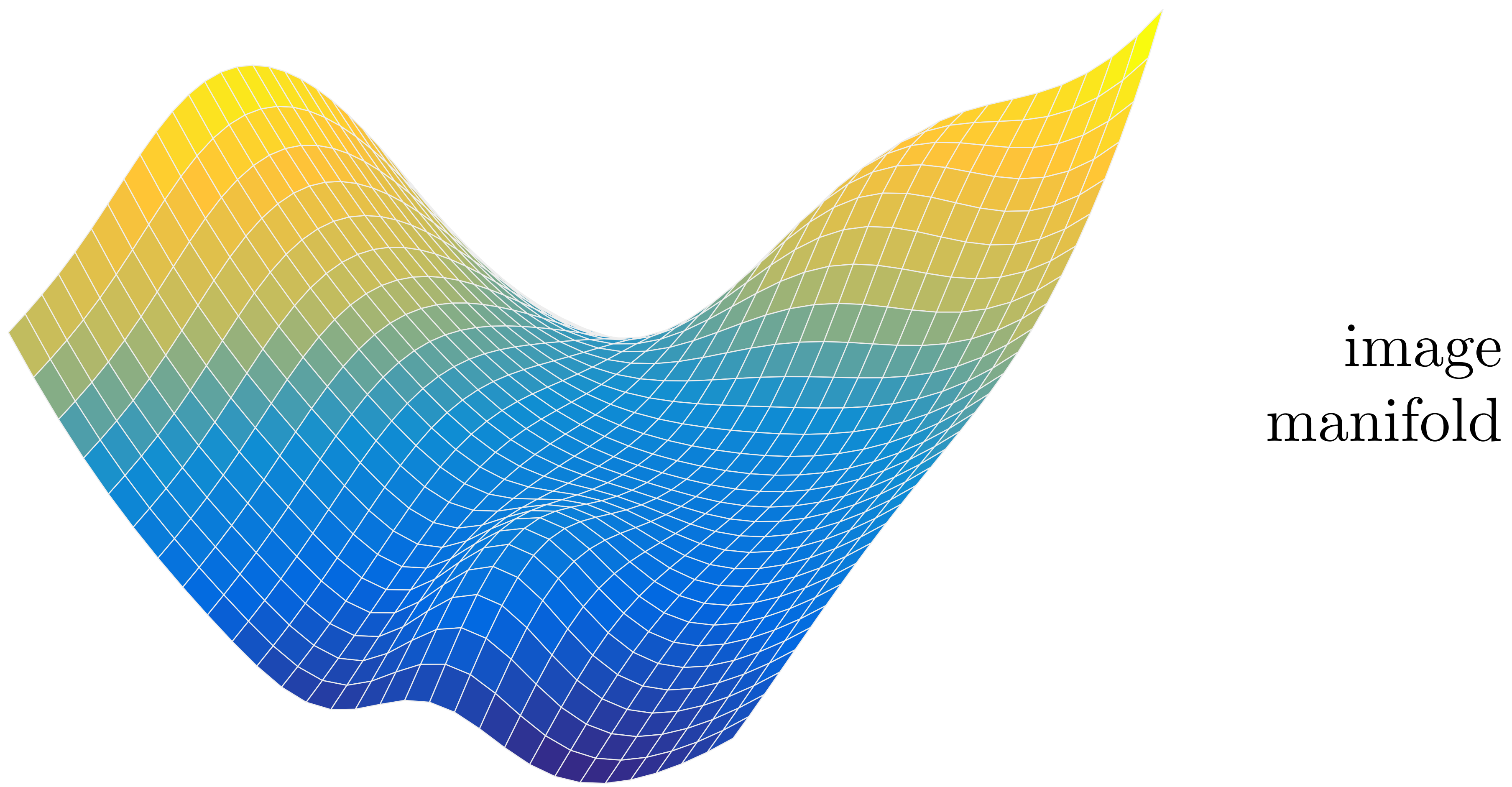
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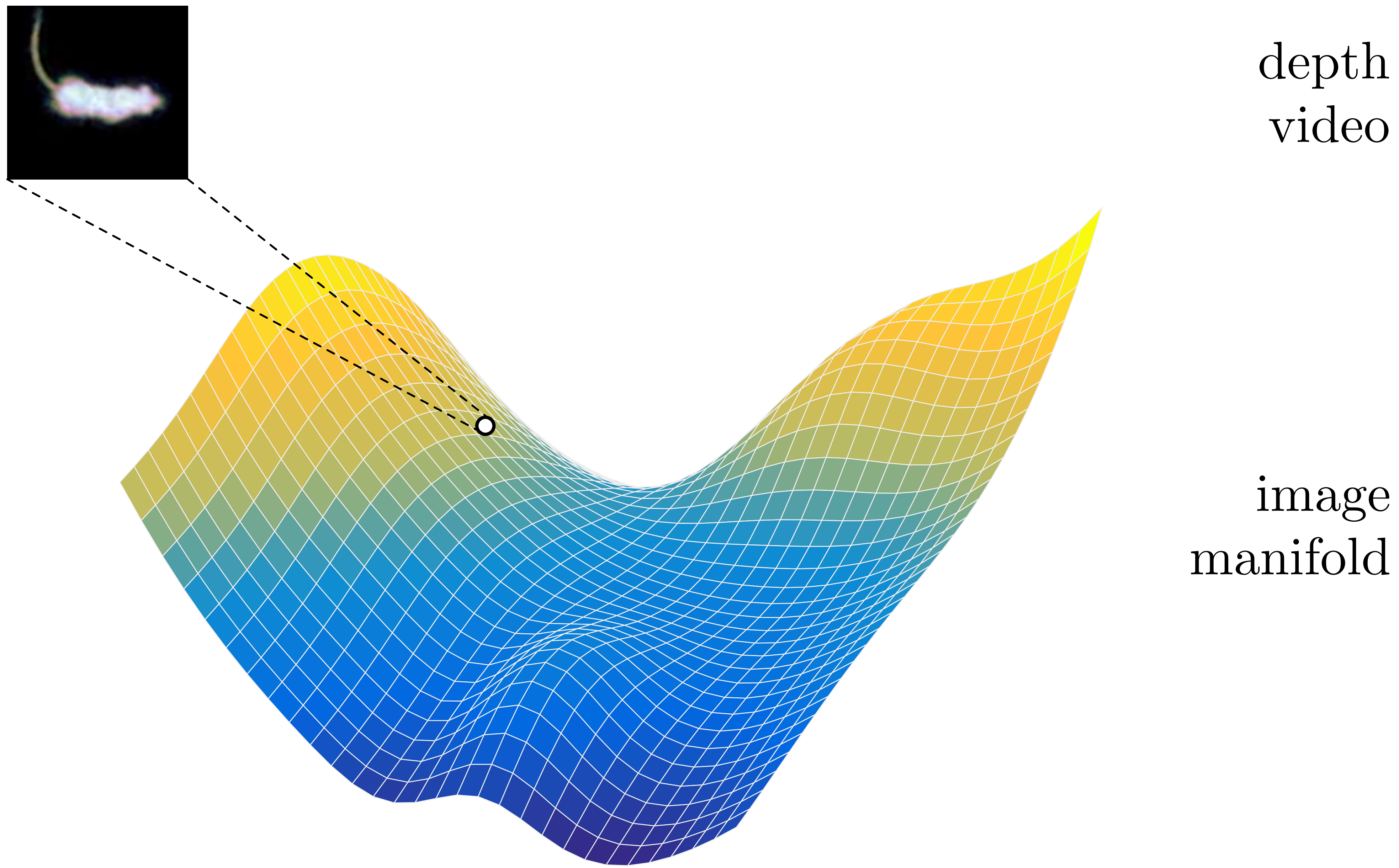
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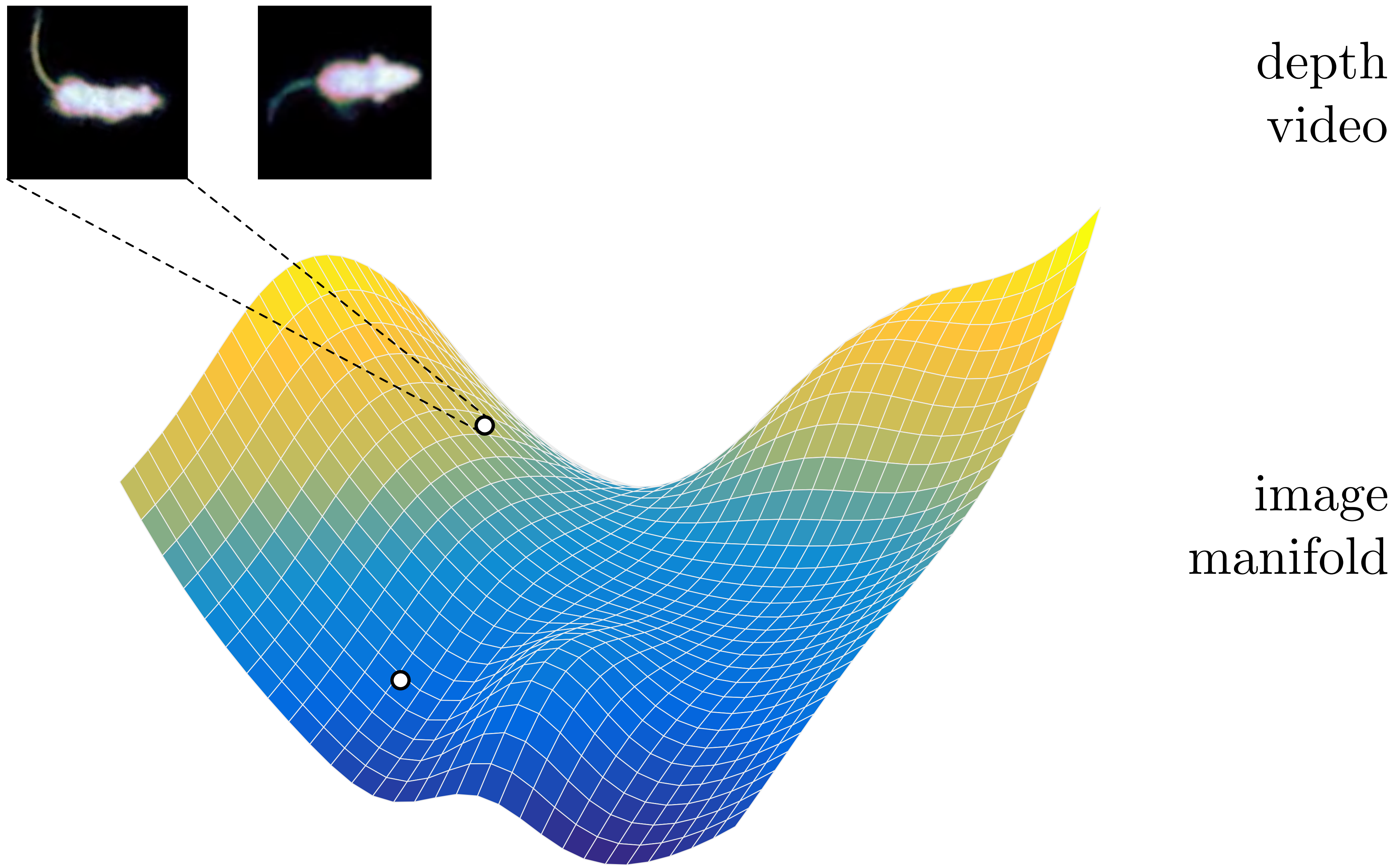
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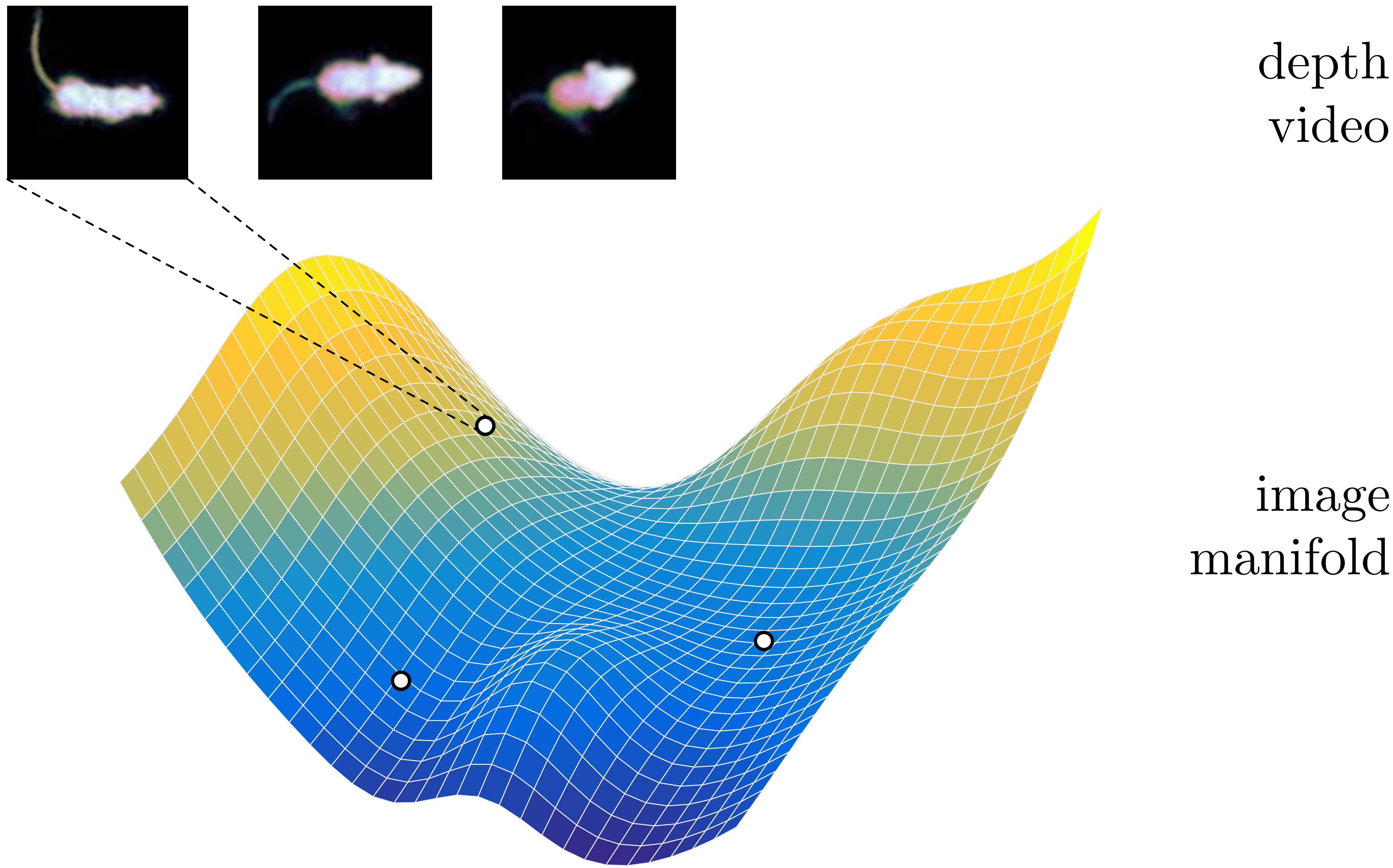
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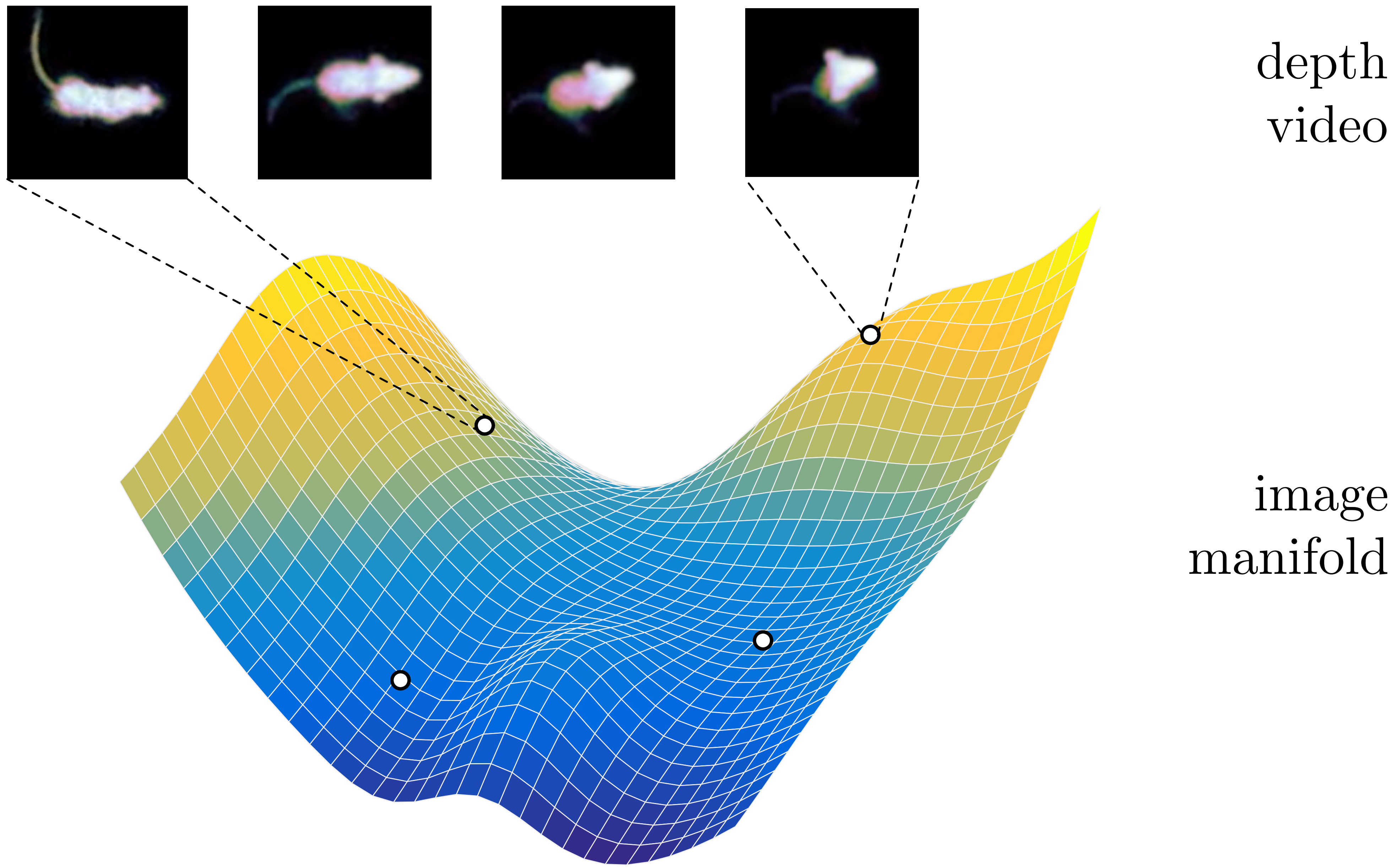
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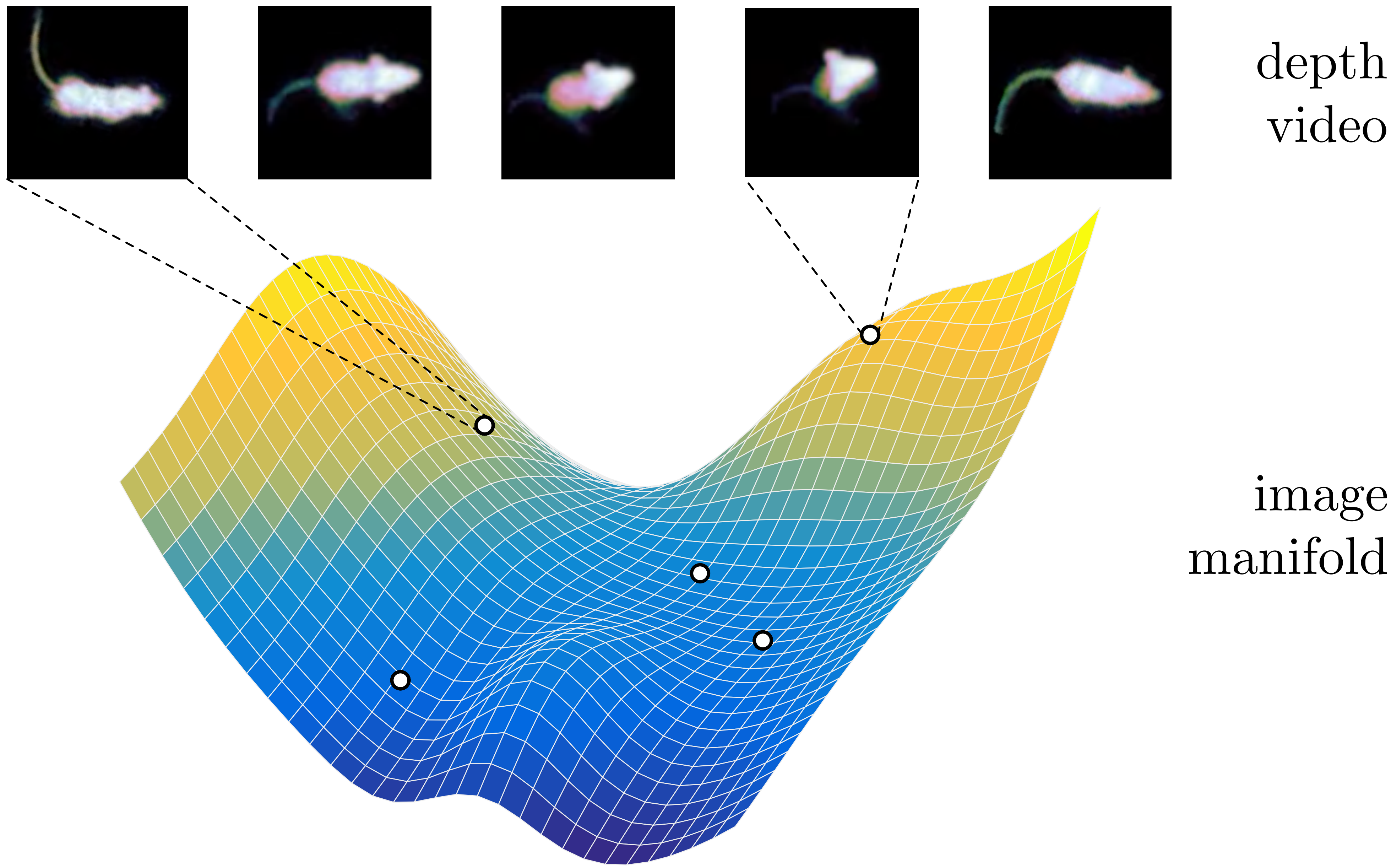
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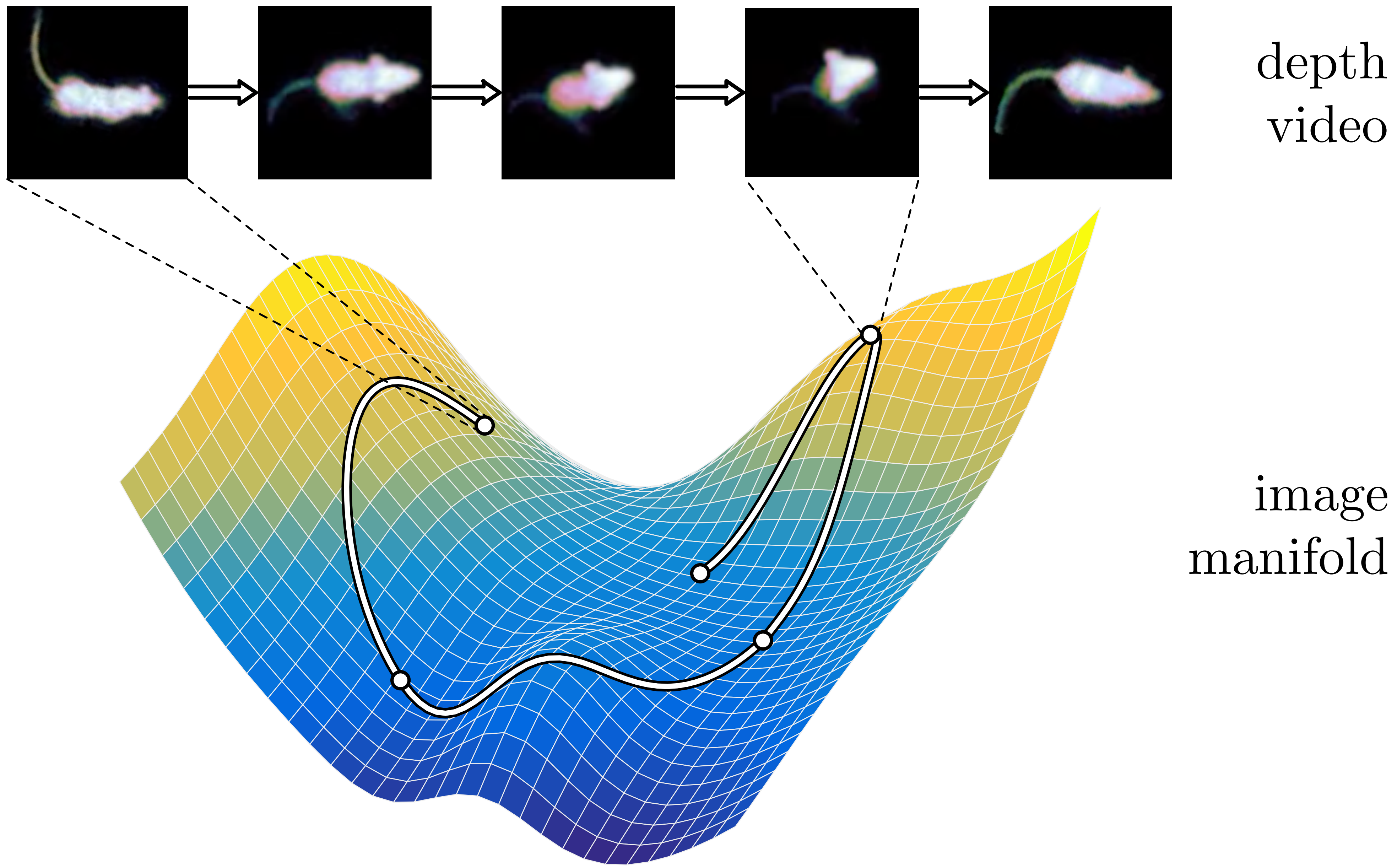
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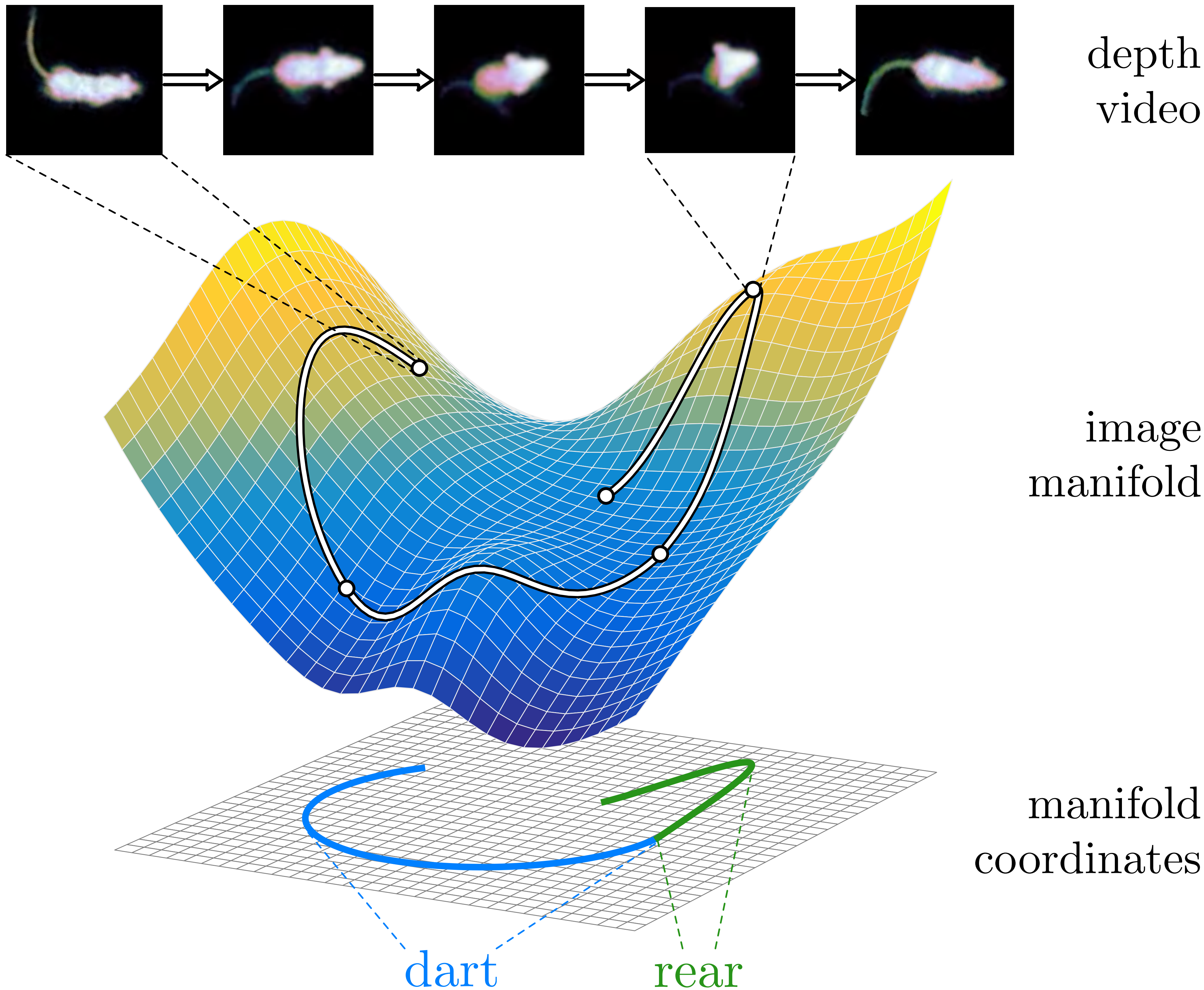
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Recurrent neural networks? [1,2,3]

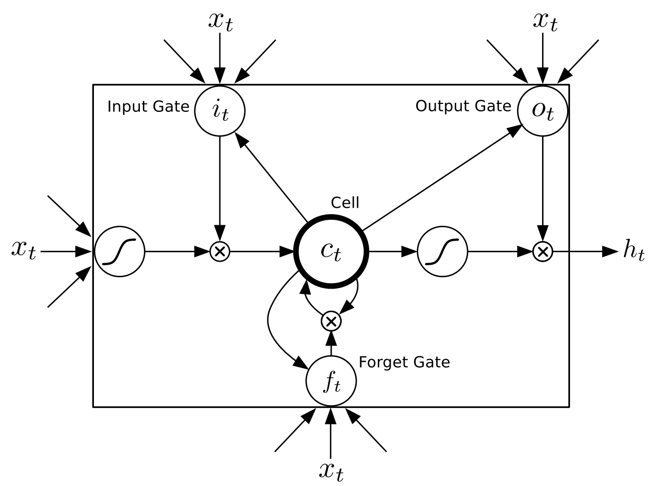

Figure 1. LSTM unit

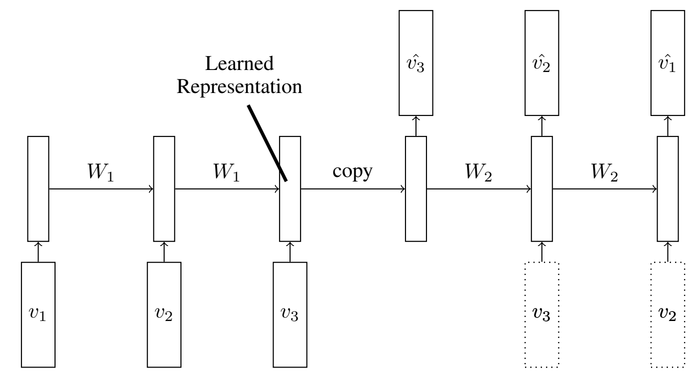

Figure 2. LSTM Autoencoder Model

[1] Srivastava, Mansimov, Salakhutdinov. Unsupervised learning of video representations using LSTMs. ICML 2015.
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[3] Sutskever, Hinton, and Taylor. The Recurrent Temporal Restricted Boltzmann Machine. NIPS 2008.

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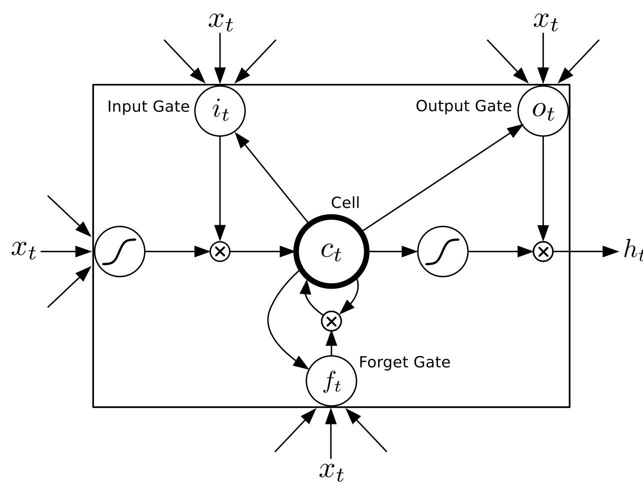

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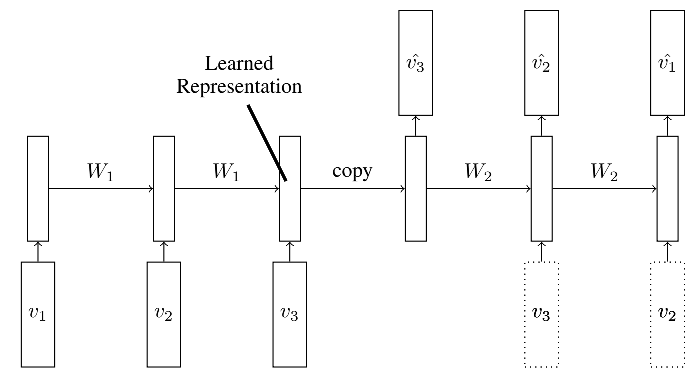

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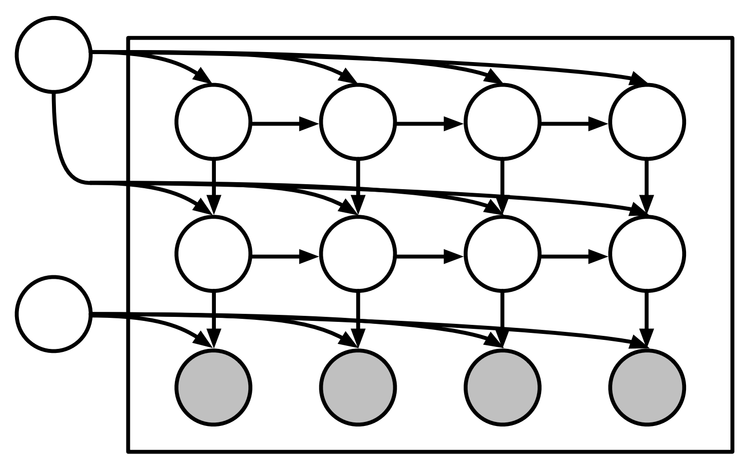
Probabilistic graphical models? [4,5,6]



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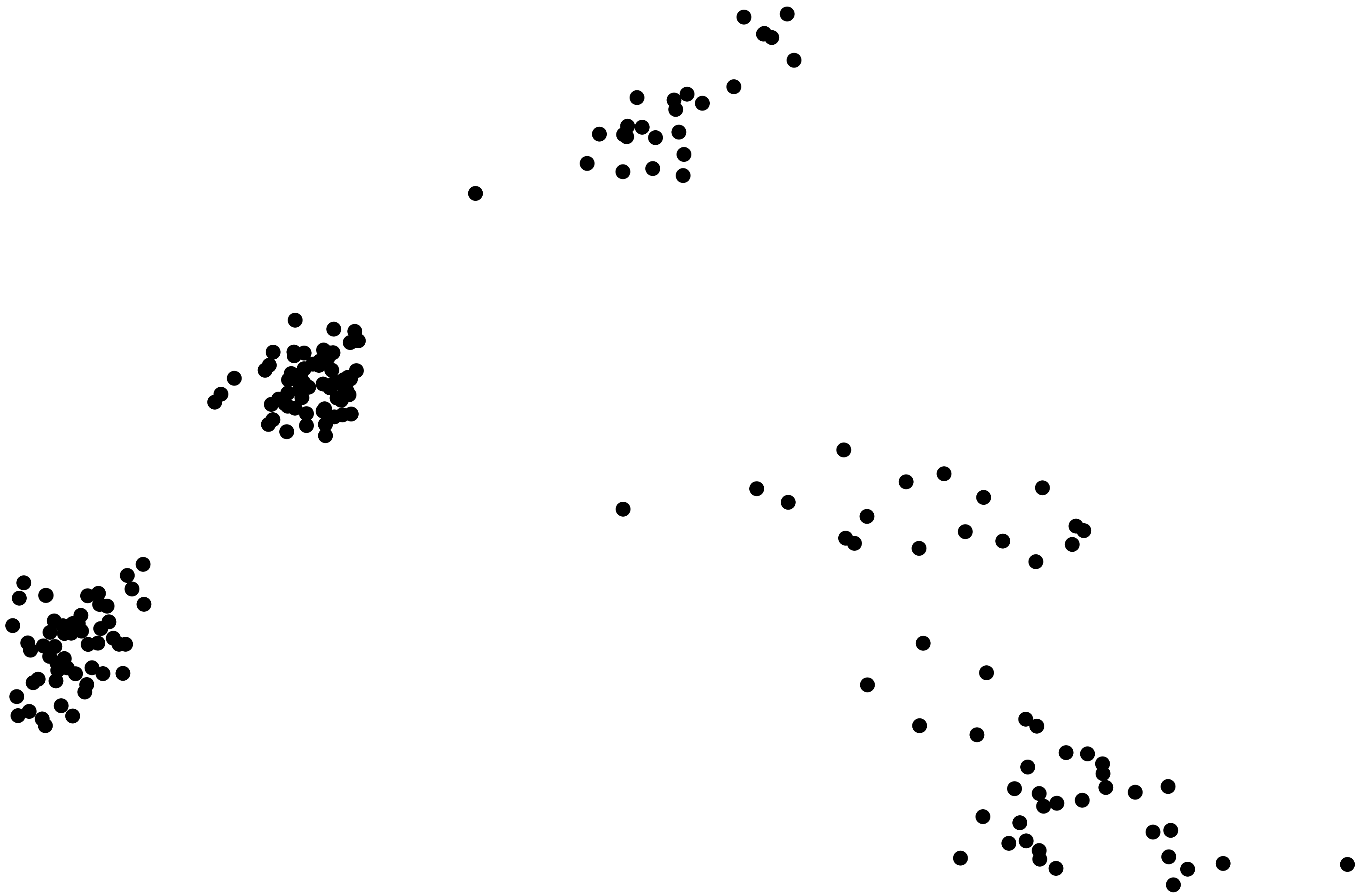
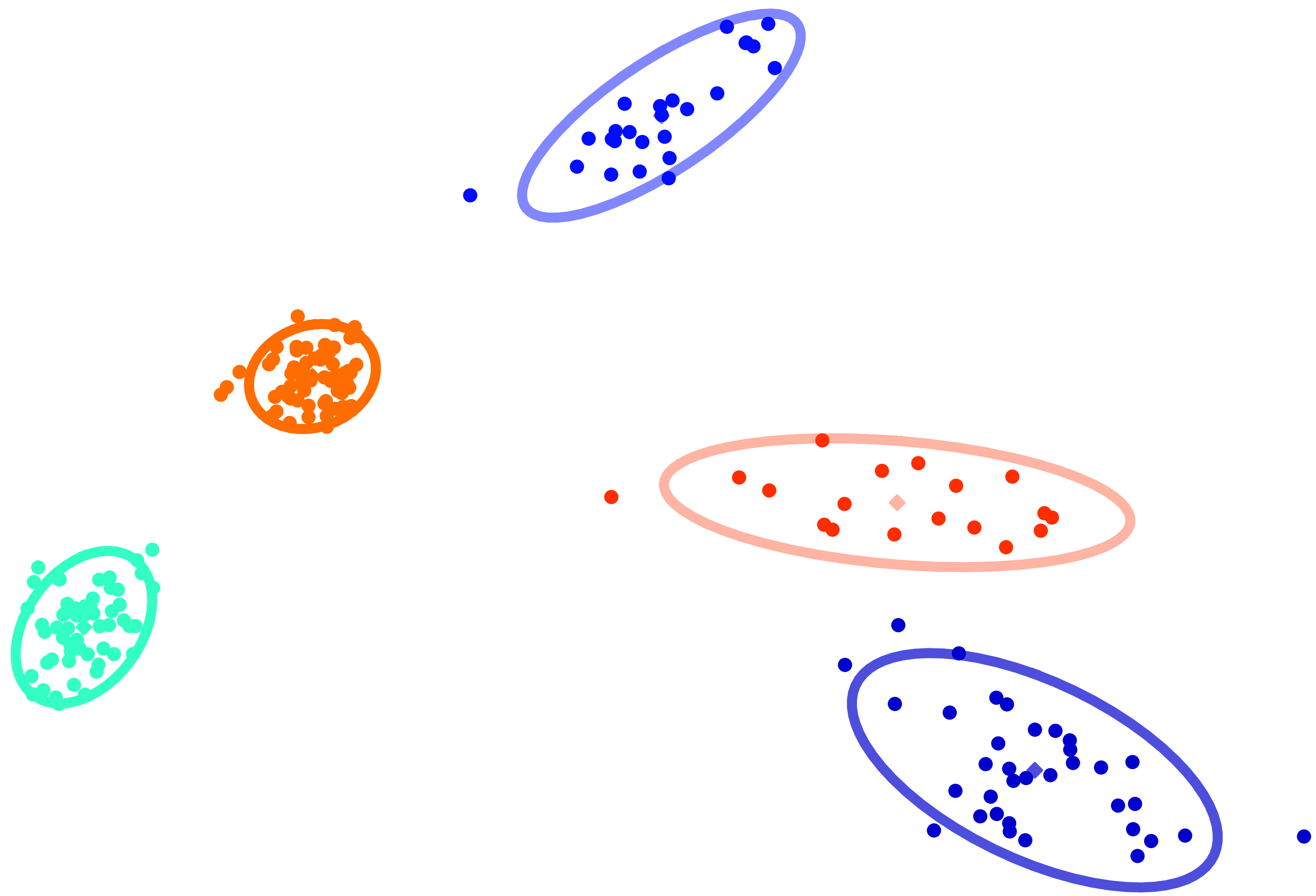
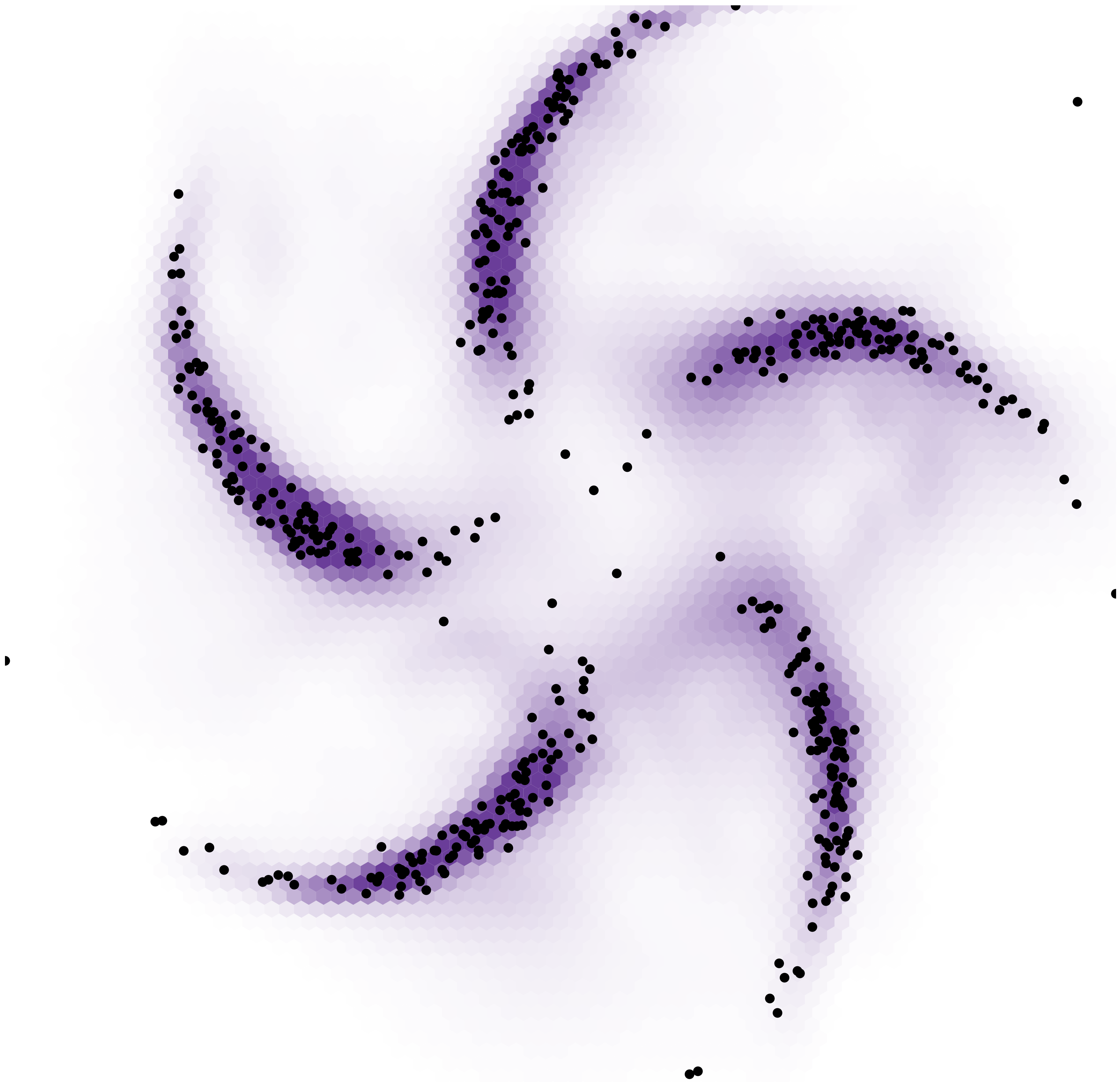
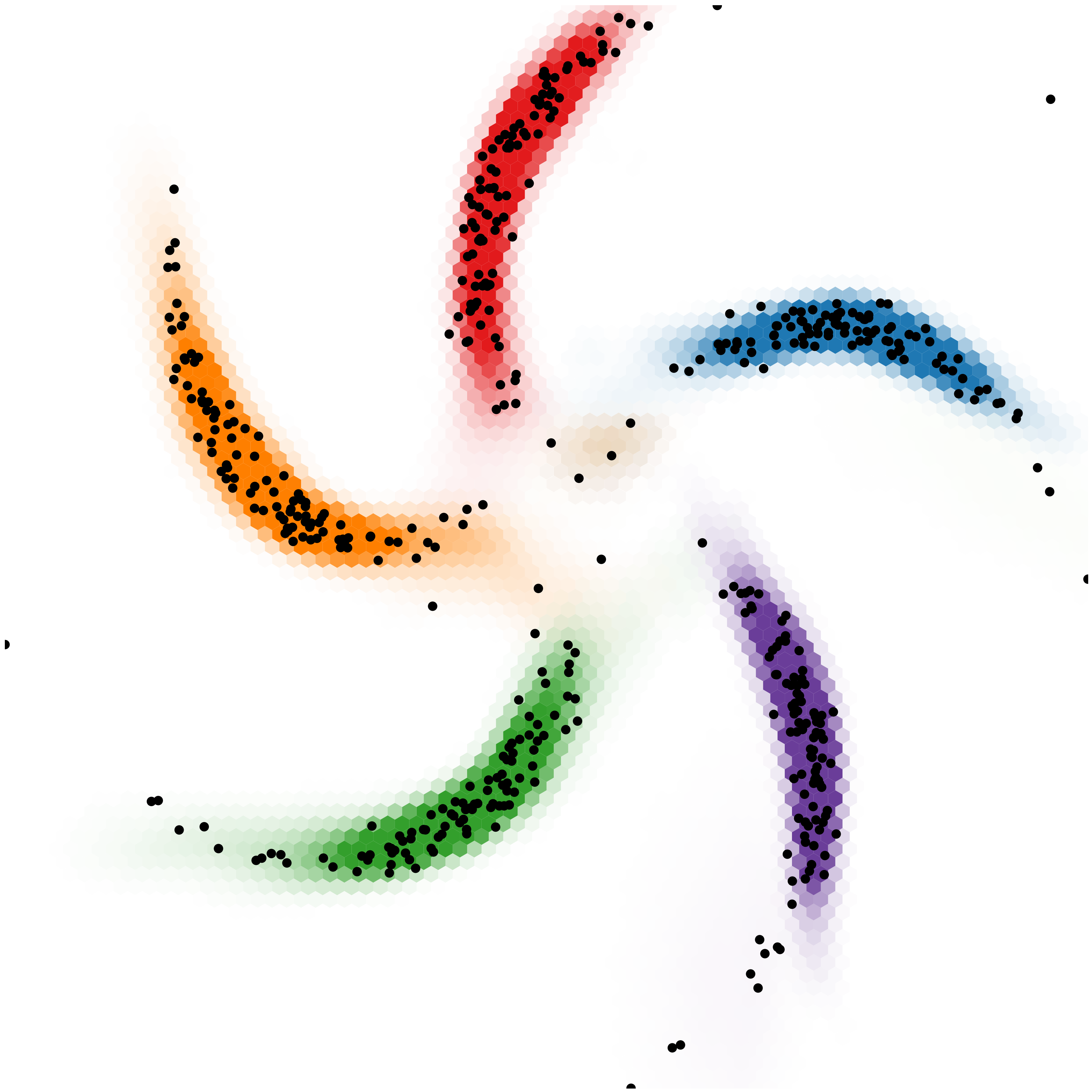
[4] Fox, Sudderth, Jordan, Willsky. Bayesian nonparametric inference of switching dynamic linear models. IEEE TSP 2011.
[5] **Johnson** and Willsky. Bayesian nonparametric hidden semi-Markov models. JMLR 2013.
[6] Murphy. Machine learning: a probabilistic perspective. MIT Press 2012.

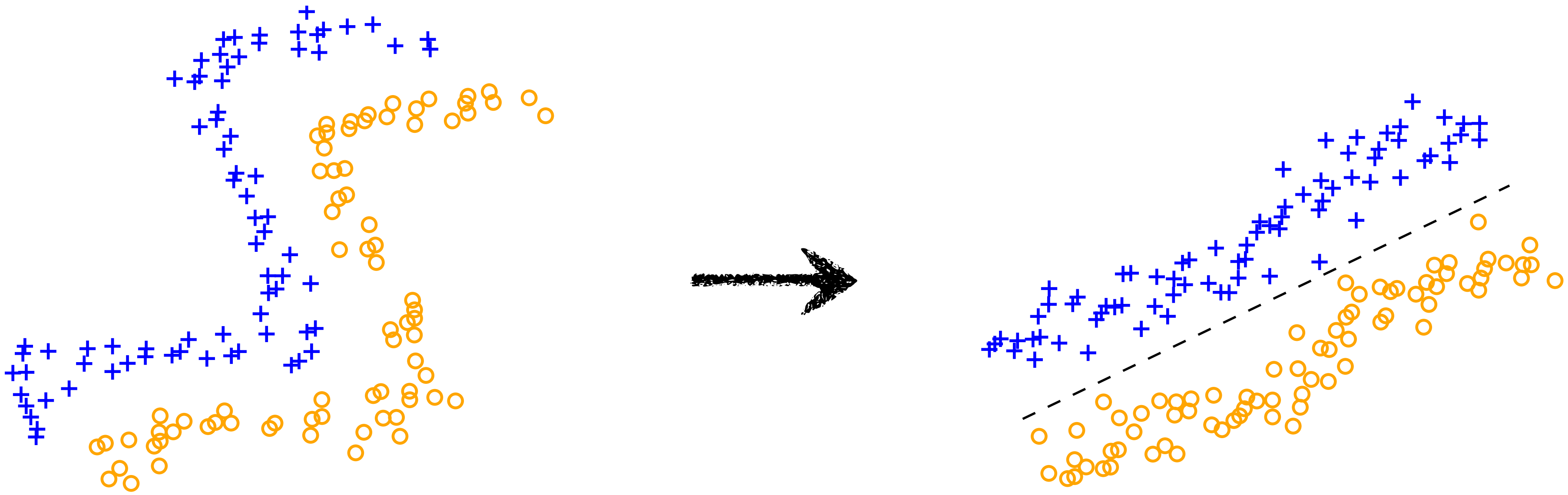




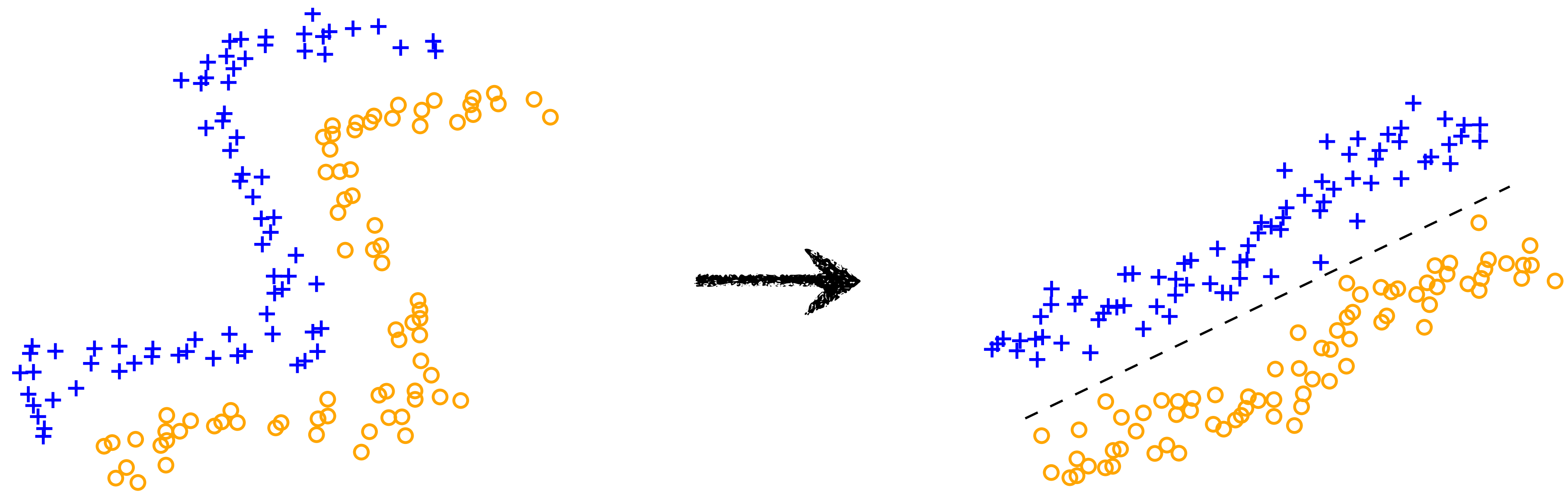




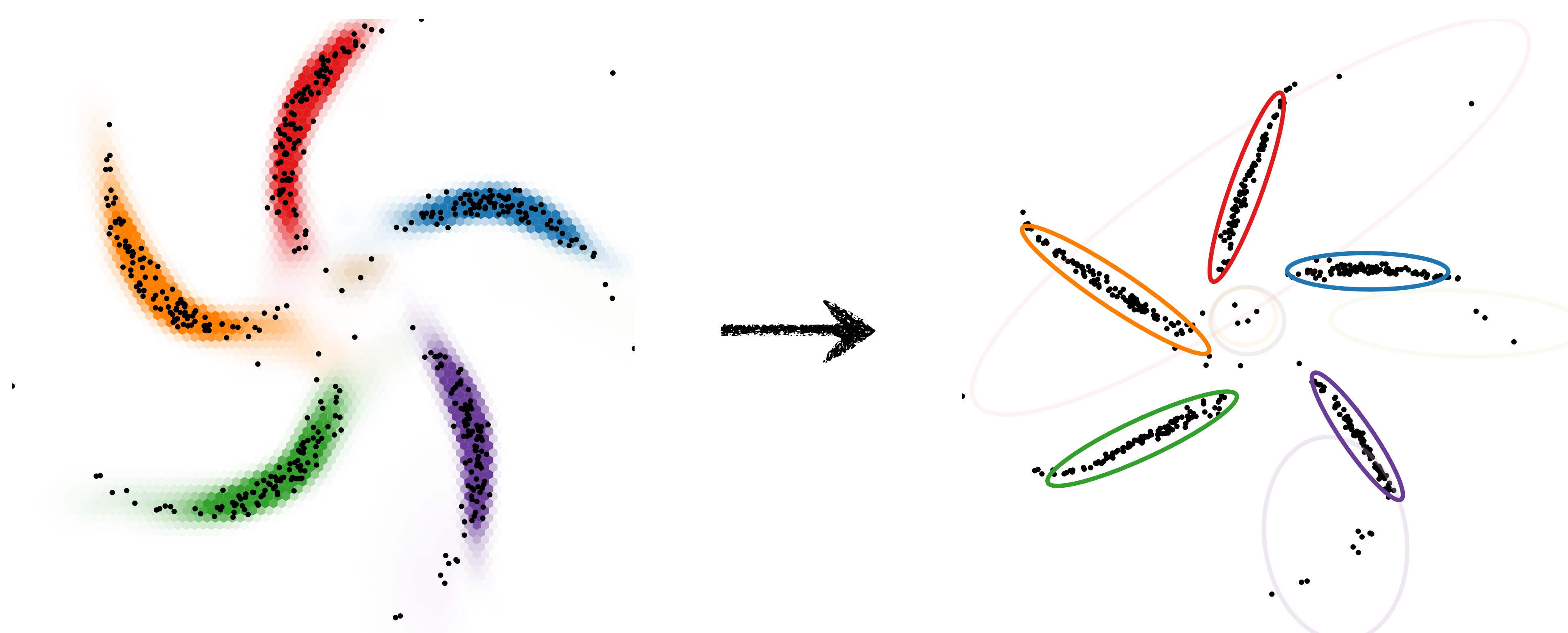
supervised
learning



supervised learning



unsupervised learning



Probabilistic graphical models

Deep learning

Probabilistic graphical models

+ structured representations
+ priors and uncertainty
– rigid assumptions may not fit
– feature engineering

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Probabilistic graphical models | Deep learning

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Deep learning

– neural net "goo"
– difficult parameterization
+ flexible, high capacity
+ feature learning

– limited inference queries
– data- and compute-hungry
+ recognition networks learn how to do inference

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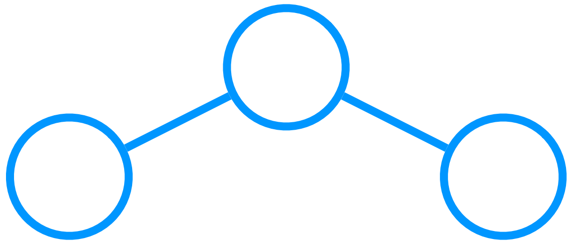
Graphs



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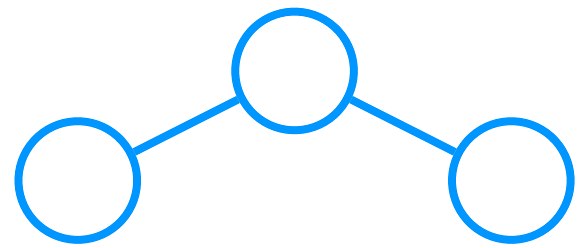
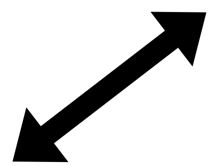
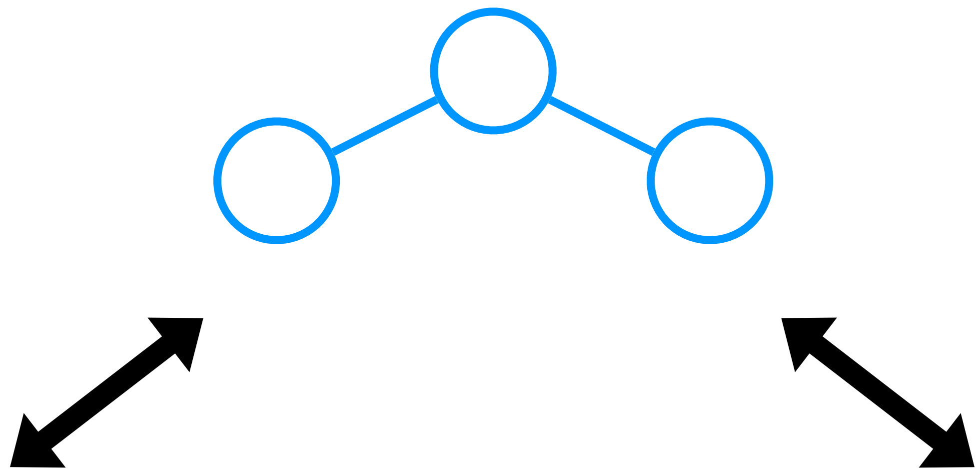




Independence of RVs

$$X_1 \perp\!\!\!\perp X_3 \mid X_2$$

Graphs



Independence of RVs

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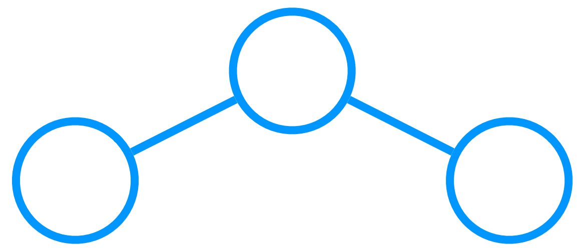
Algebraic structure in density

$$p(x) = \frac{1}{Z} \prod_C \psi_C(x_C)$$

Graphs



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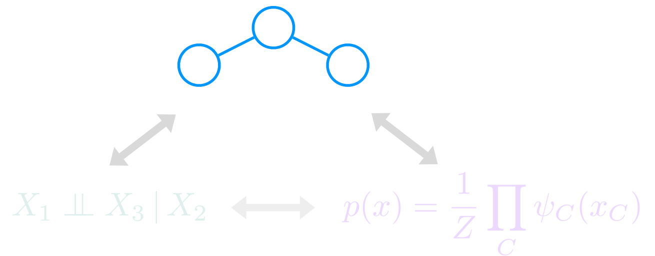
$$G = (V, E)$$

$$V = \{1, 2, \ldots, n\}$$

$$E \subseteq \{ \, \{u, v\} : u, v \in V \, \}$$



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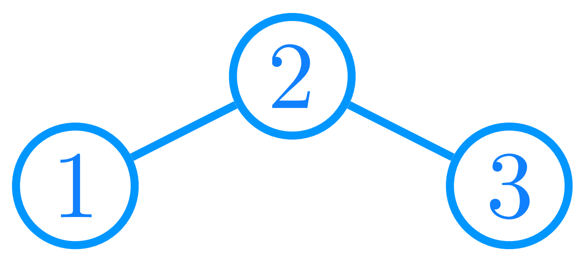
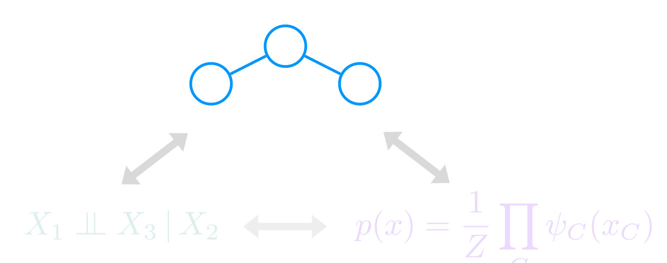
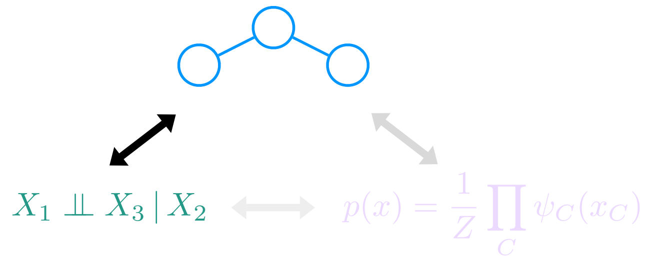


$$V = \{1, 2, 3\}$$

$$E = \{\, \{1, 2\}, \{2, 3\} \,\}$$



Def $X = \{X_v\}_{v \in V}$ is *Markov on* G iff for disjoint $A, B, C \subseteq V$ when C disconnects A from B we have $X_A \perp\!\!\!\perp X_B \,|\, X_C$.



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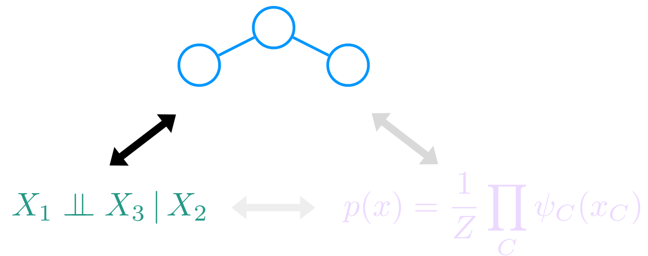
<u>disconnects</u> means no path from A to B after removing C.



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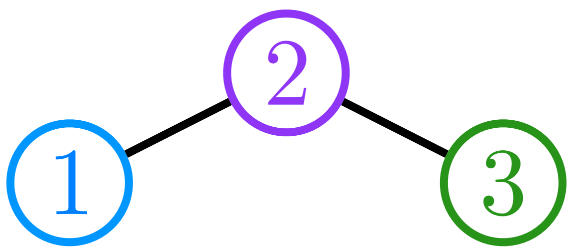
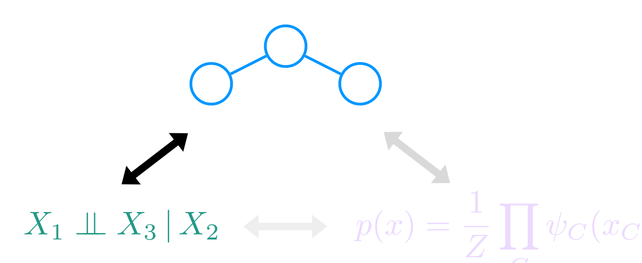


$$\Longrightarrow \qquad X_1 \perp\!\!\!\perp X_3 \,|\, X_2$$



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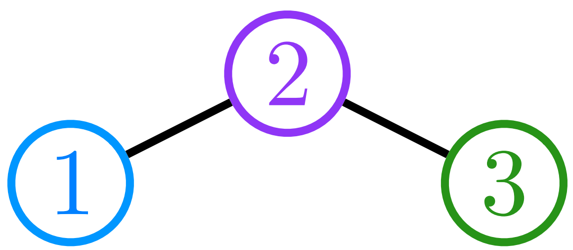

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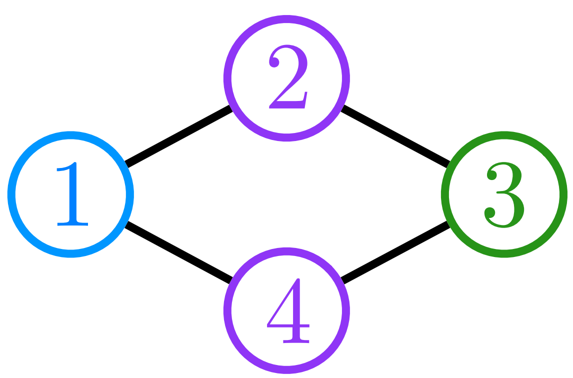
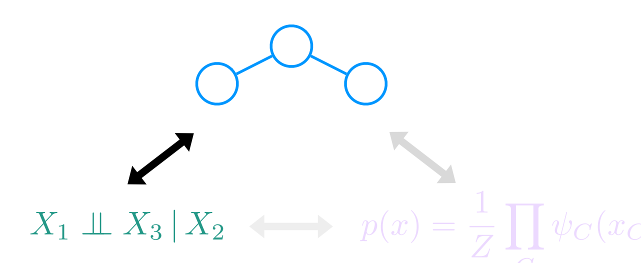


$$\implies \qquad X_1 \perp\!\!\!\perp X_3 \,|\, X_2, X_4$$



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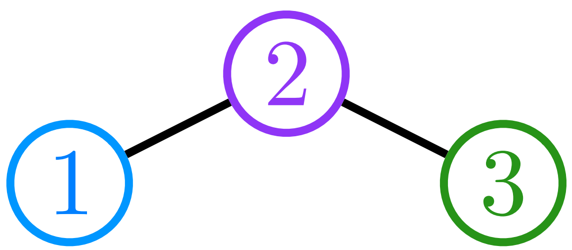
<u>disconnects</u> means no path from A to B after removing C.



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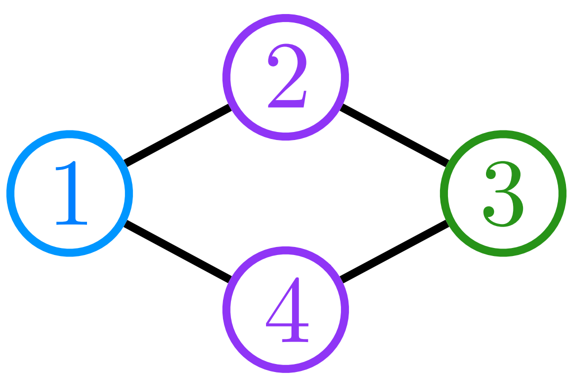

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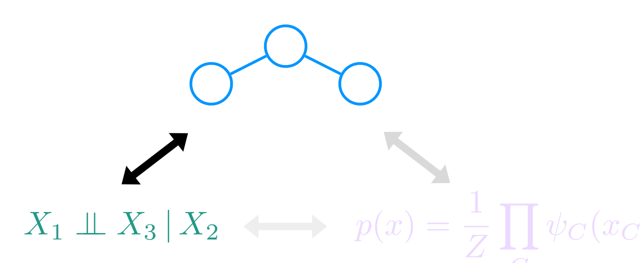

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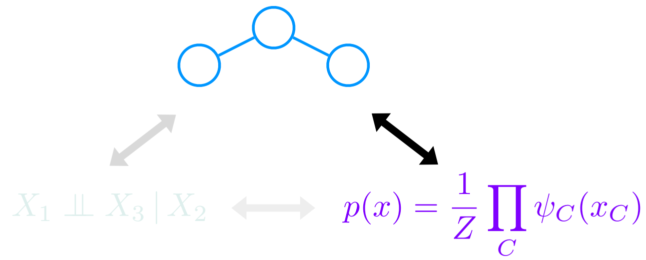

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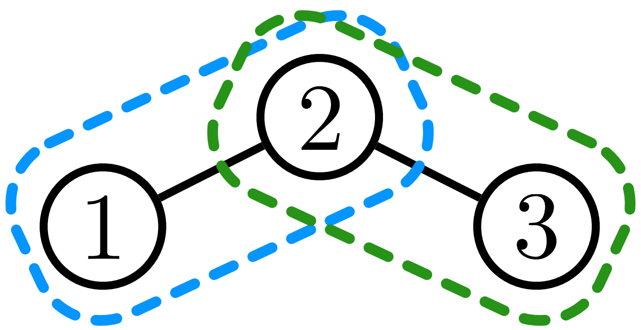
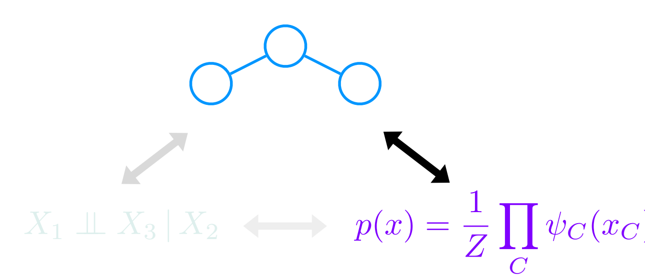


$$\Longrightarrow \quad p(x) \propto \psi_{12}(x_1, x_2)\psi_{23}(x_2, x_3)$$



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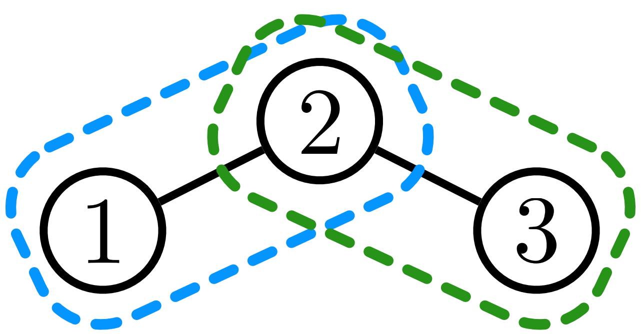

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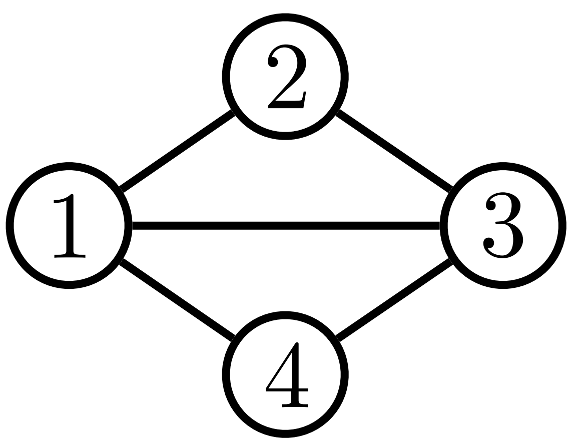

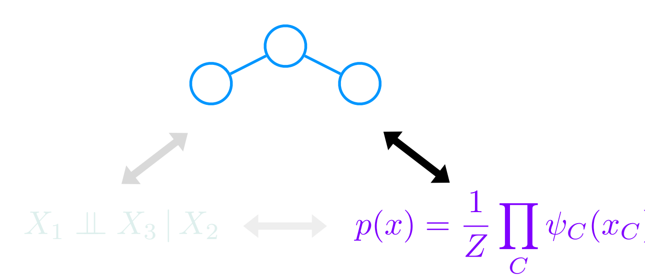

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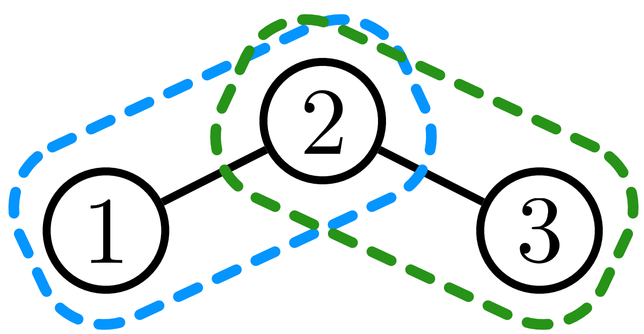

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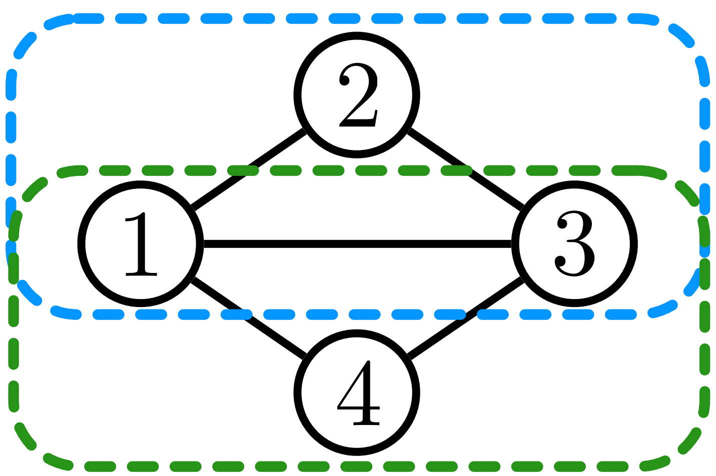
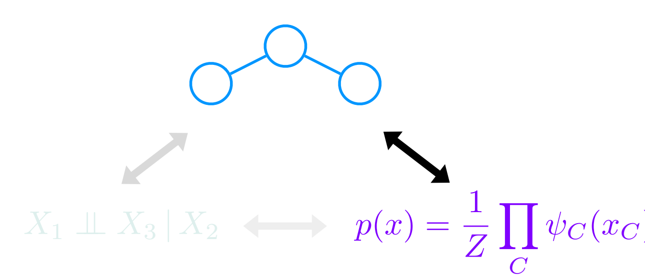


$$\Longrightarrow \quad p(x) \propto \psi_{123}(x_1, x_2, x_3)\psi_{134}(x_1, x_3, x_4)$$



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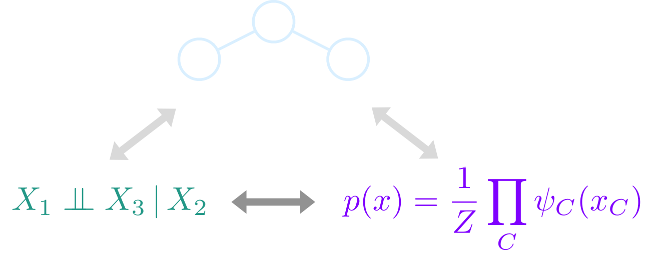

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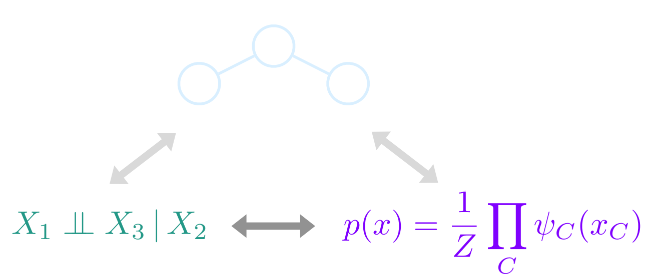
$$\text{Markov on } G \quad \not\Longleftrightarrow \quad \text{factorizes on } G$$



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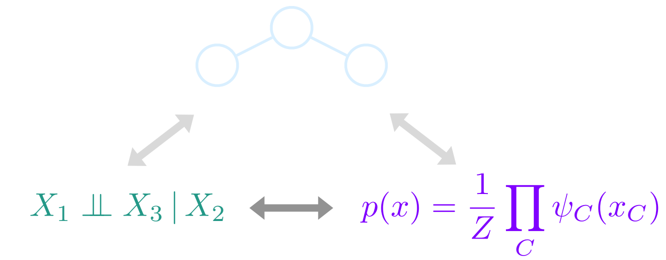
Markov on G $\quad \not\Longleftrightarrow \quad$ factorizes on G

... but they are the same if $p(x) > 0$.



A good way to ensure $p(x) > 0$ is to have $p(x) = \exp(-E(x))$.

$$p(x) = \frac{1}{Z} \prod_C \psi_C(x_C)$$

$$E(x) = \log Z + \sum_C \phi_C(x_C)$$

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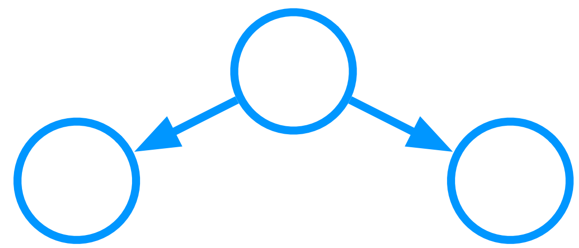
$$E(x; \eta) = \log Z + \sum_{C} \eta_C \cdot \phi_C(x_C)$$

Graphs



Independence of RVs

$$X_1 \perp\!\!\!\perp X_3 \mid X_2$$

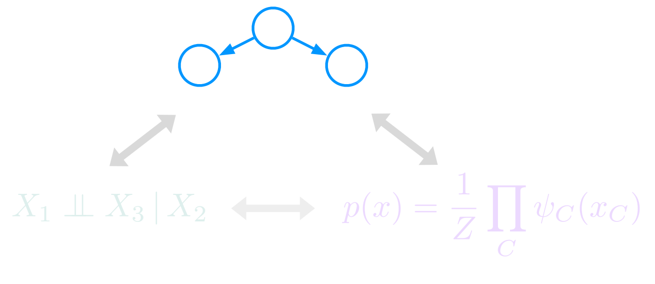
Algebraic structure in density

$$p(x) = \prod_{v \in V} p(x_v \mid x_{\mathrm{pa}(v)})$$

$$G = (V, E)$$

$$V = \{1, 2, \ldots, n\}$$

$$E \subseteq V \times V$$



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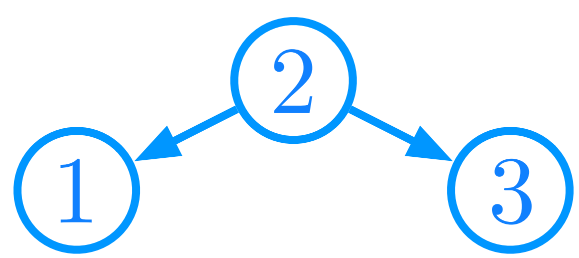
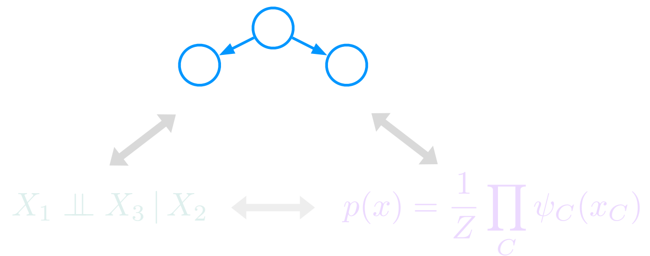


$$V = \{1, 2, 3\}$$

$$E = \{\ (2, 1),\ (2, 3)\ \}$$



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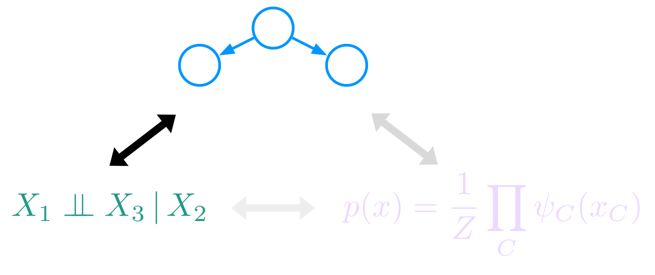
d-separates means no unblocked undirected path from A to B.



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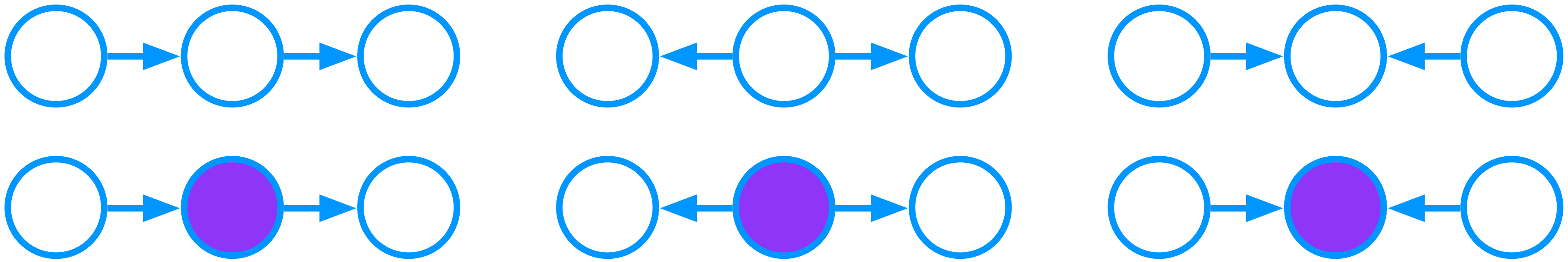

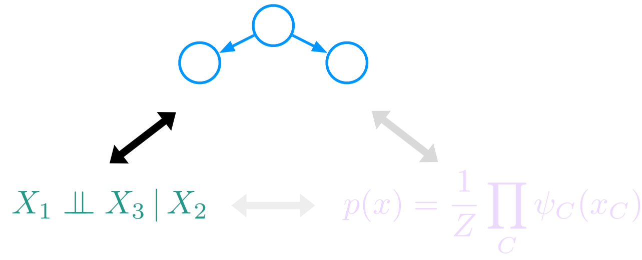

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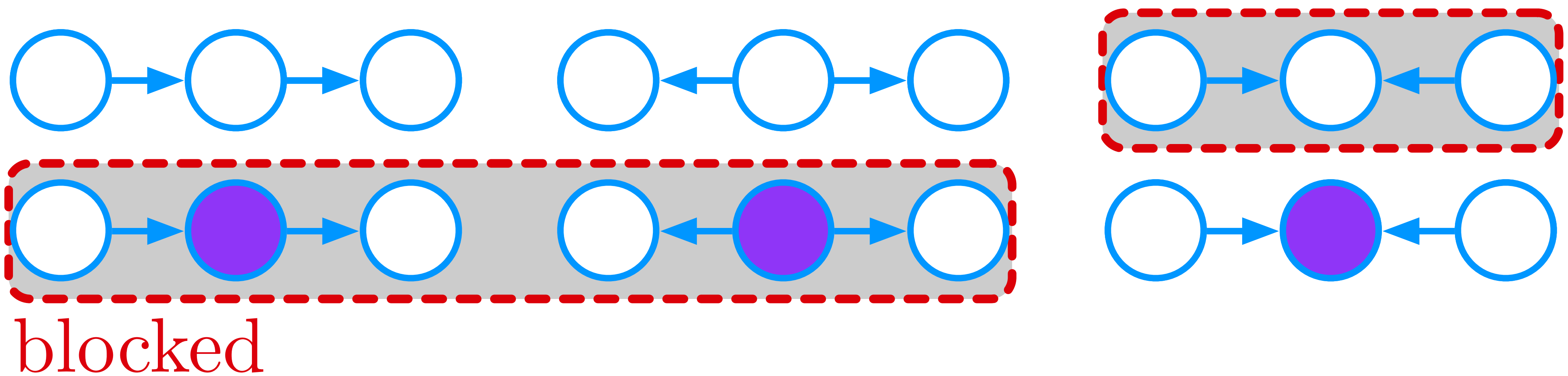

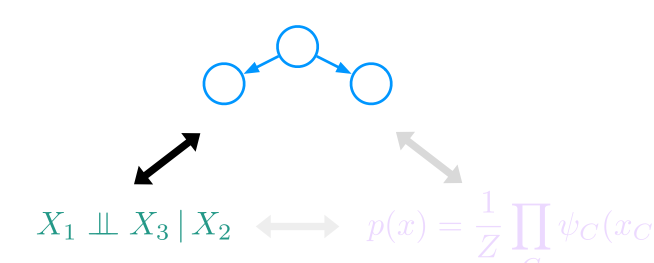

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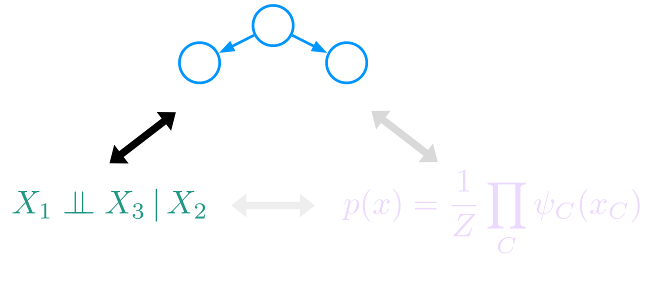

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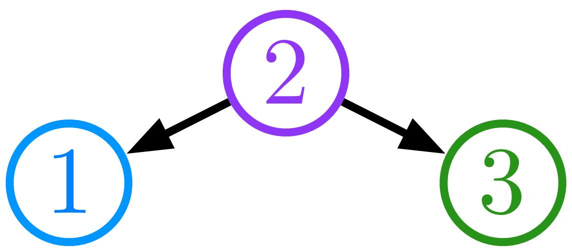

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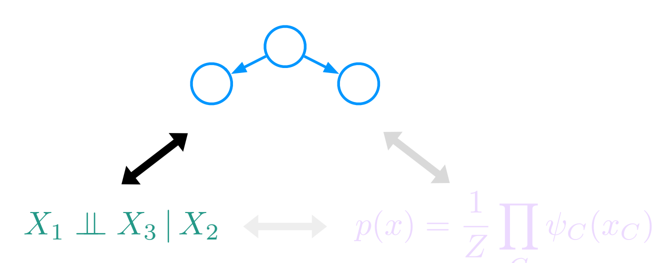

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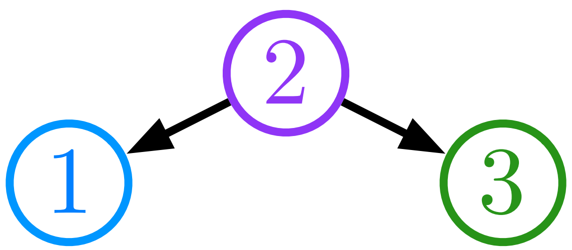

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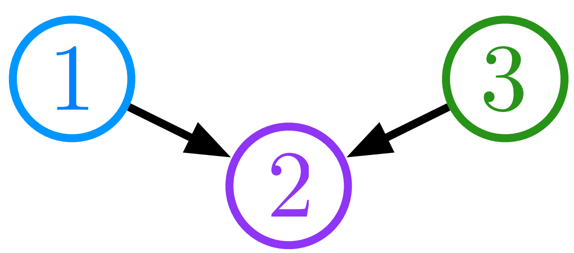

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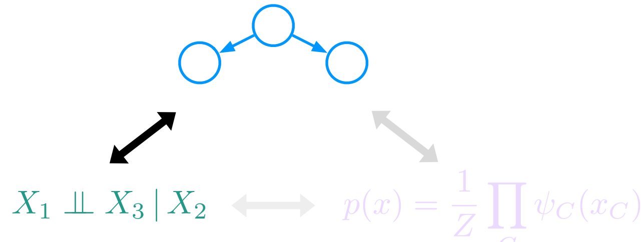

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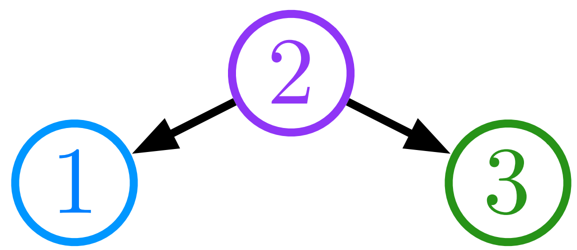

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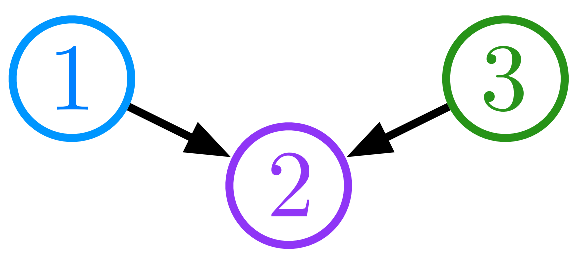

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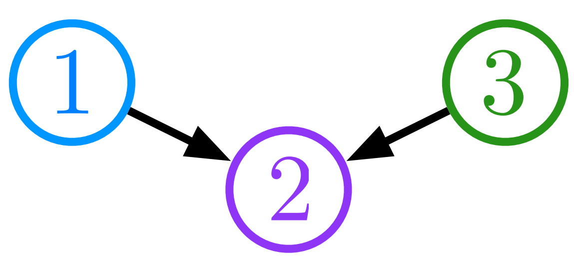

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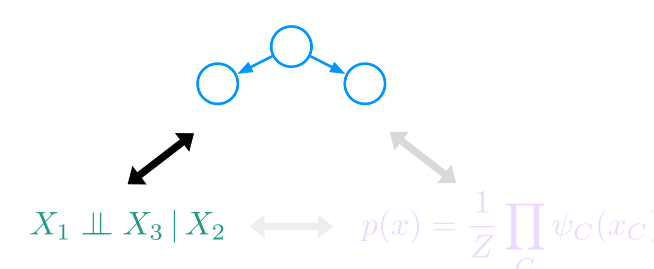

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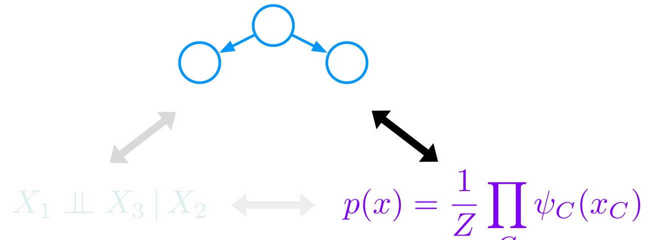

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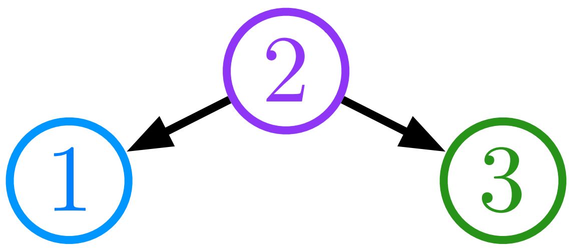
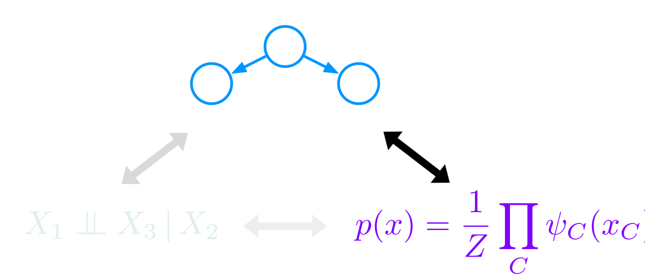


$$\Longrightarrow \quad p(x) = p(x_2)p(x_1 \mid x_2)p(x_3 \mid x_2)$$



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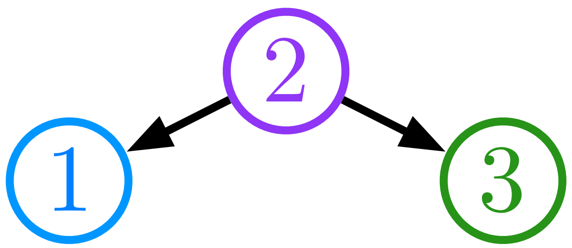

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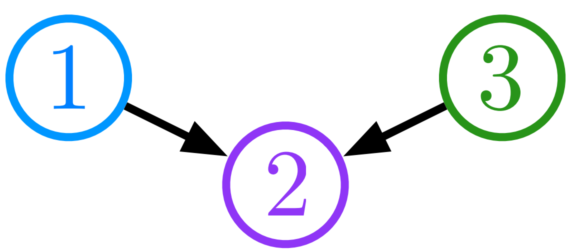

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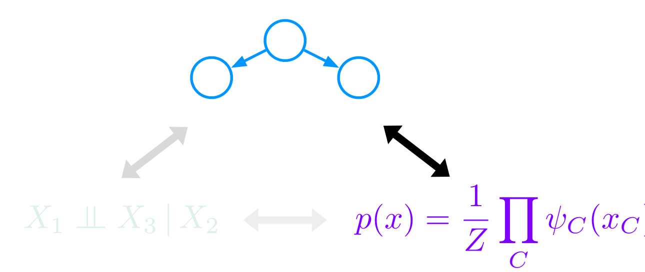
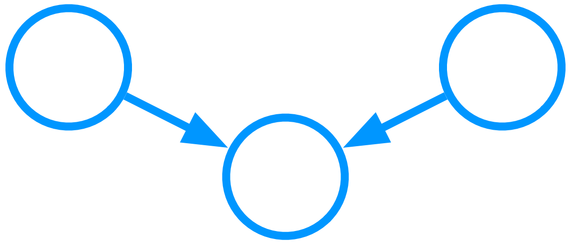
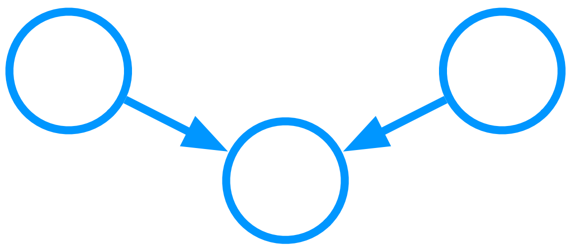




Directed models often appear with generative models

- Ancestral sampling
- For Gaussians, like having a Cholesky factorization



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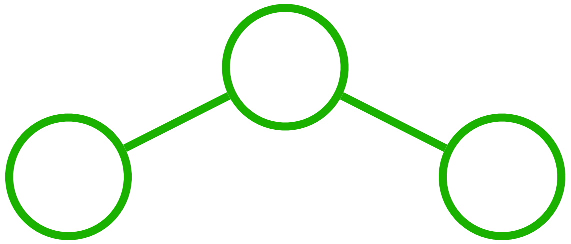
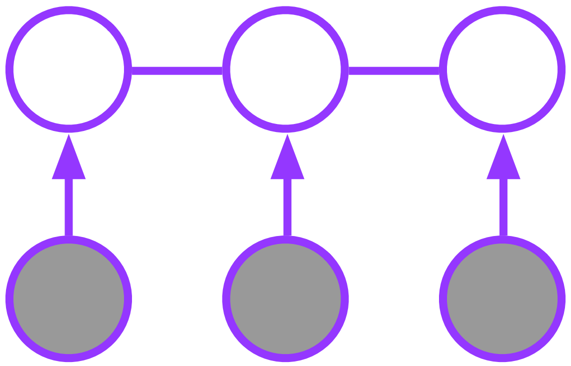


Undirected models often appear in inference

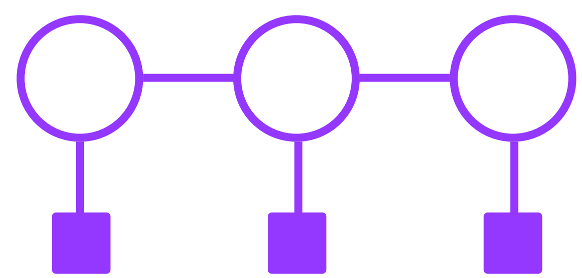
- For Gaussians, like solving the linear system

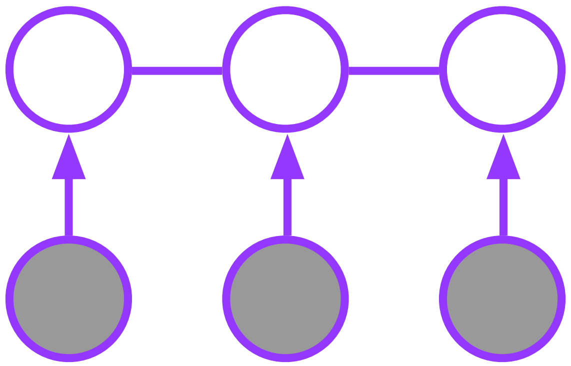
$$J\mu = h$$



Conditional random fields (CRFs) are PGMs where potentials depend on exogenous data

$$p(y\,;\,x) \propto \psi_1(y_1\,;\,x_1)\psi_{12}(y_1, y_2)\psi_2(y_2\,;\,x_2)\psi_{23}(y_2, y_3)\psi_3(y_3\,;\,x_3)$$





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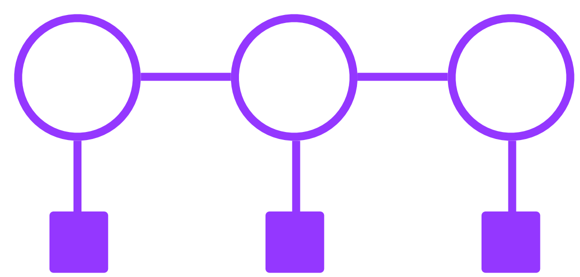
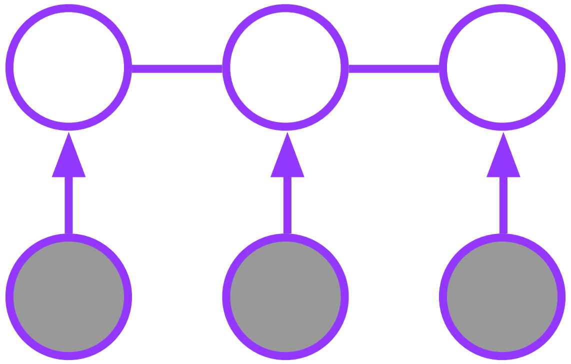


$$\psi_n(y_n\,;\,x_n) = \psi(y_n\,;\,f(x_n,\phi)) \;\; \text{for neural network} \;\; f(\,\cdot\,,\phi)$$



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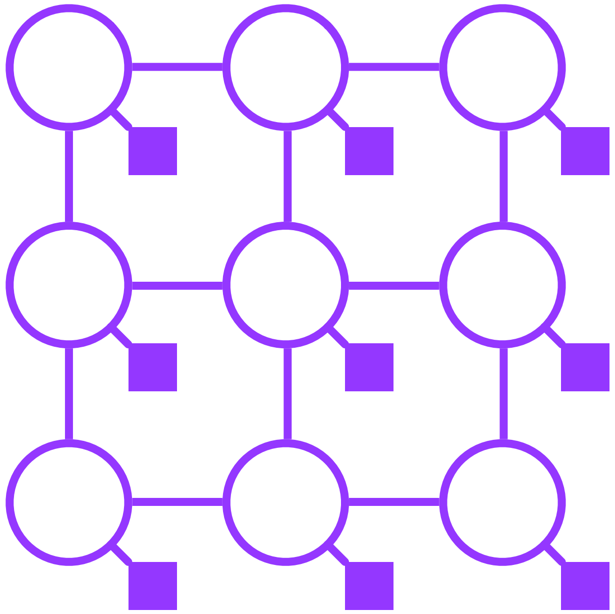

Goals

1. Motivate why PGMs + DNNs are a revolution waiting to happen
2. Survey the fundamentals of PGMs and exponential families so that you have a broad view of the territory
3. Show how to unify many models and algorithms in a framework that lets you leverage automatic differentiation
4. Make SVAEs and related PGM + DNN architectures super obvious so that you can invent better ones

Def An *exponential family of densities* is

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$$t(x)$$

defined by statistic function $t : \mathcal{X} \to W$

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defined by statistic function $t : \mathcal{X} \to \boxed{W}$ finite-dim real vector space

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Proof

$$\nabla\mathcal{A}(\eta) = \frac{1}{\int_{\mathcal{X}} \exp(\langle \eta,\, t(x)\rangle)\,\mathrm{d}x} \int_{\mathcal{X}} t(x) \exp(\langle \eta,\, t(x)\rangle)\,\mathrm{d}x$$

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Def Say family is *tractable* if $\mathcal{A}$ is easy to evaluate.

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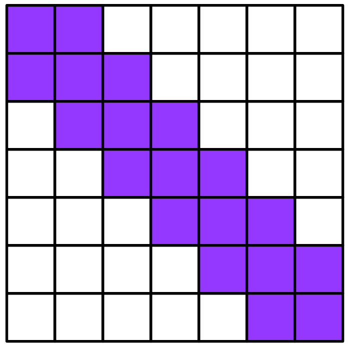

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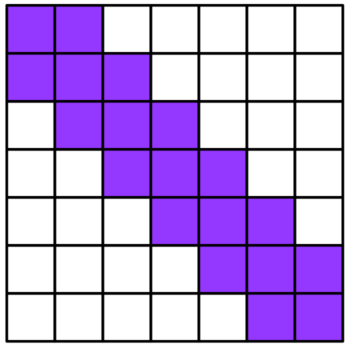

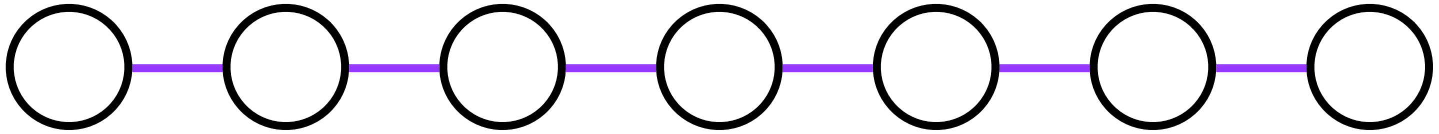

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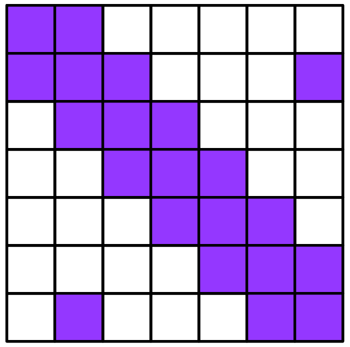

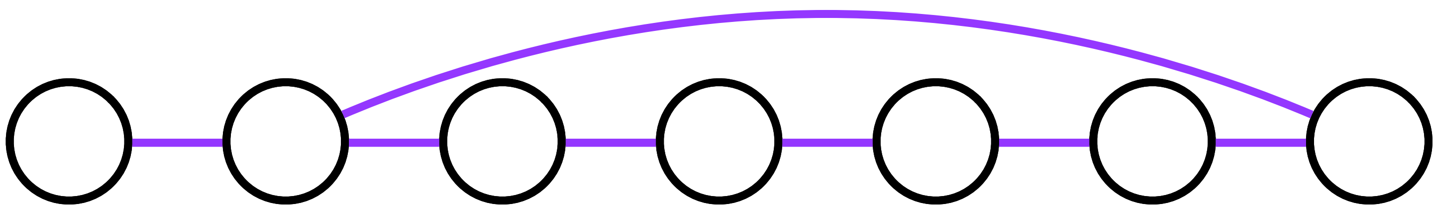

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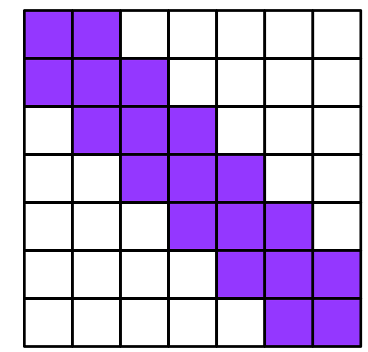
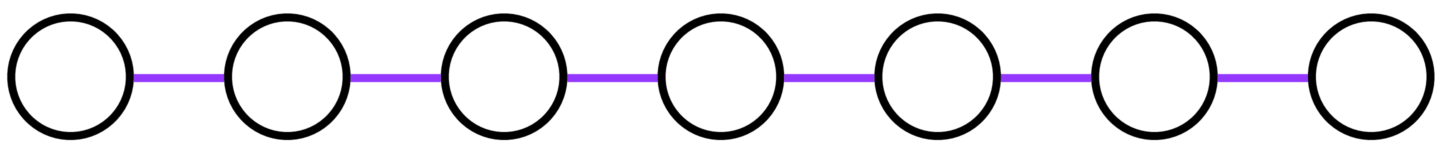
$\eta =$ 



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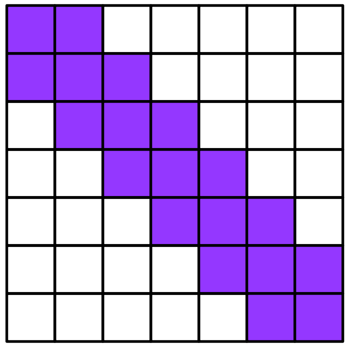
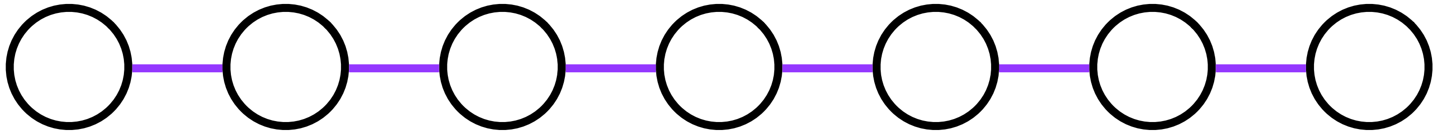
$\eta =$ 



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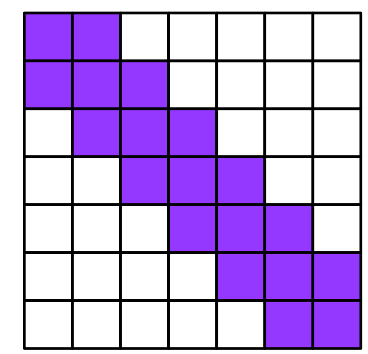

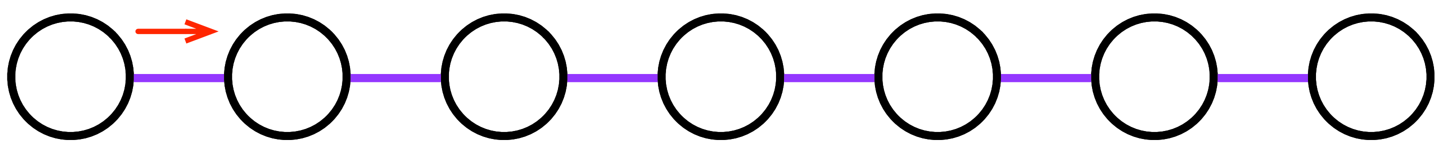

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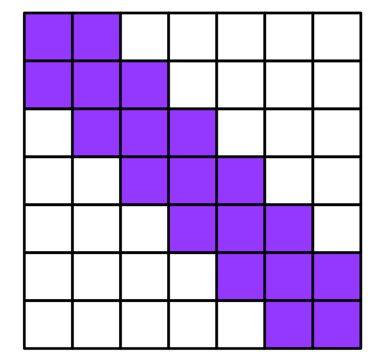

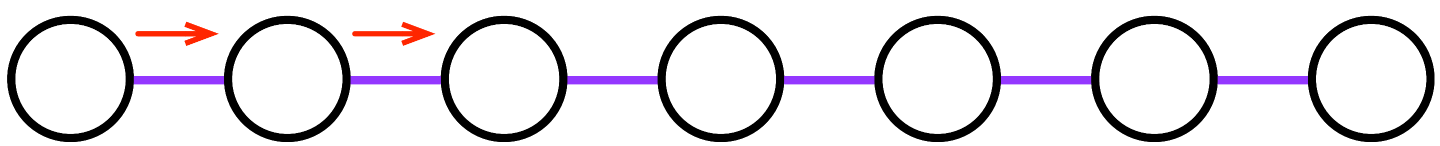

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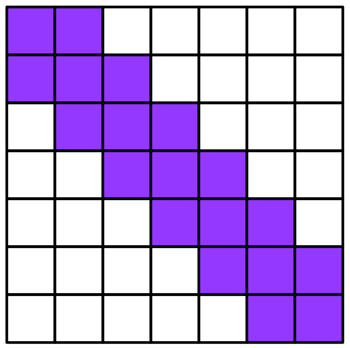

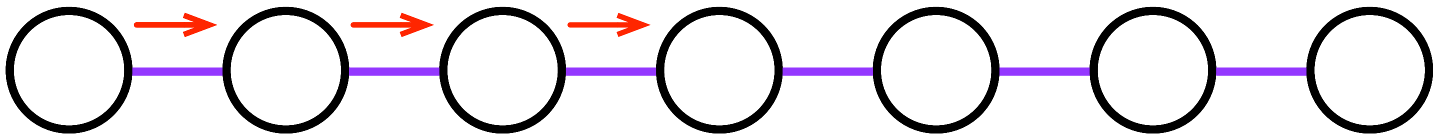

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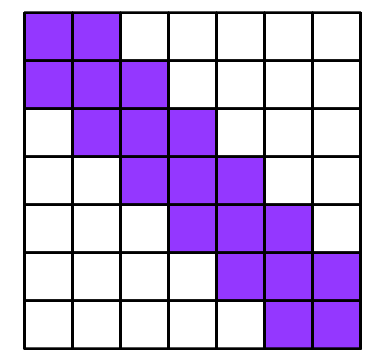

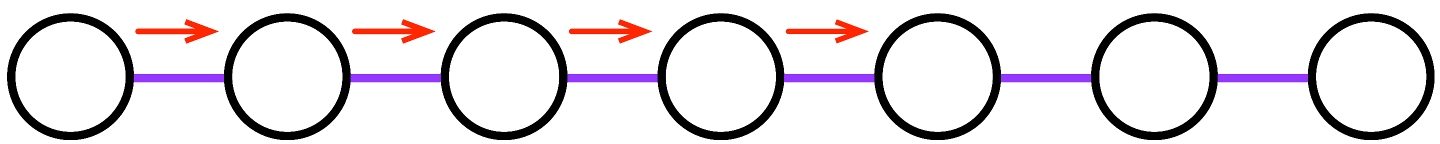

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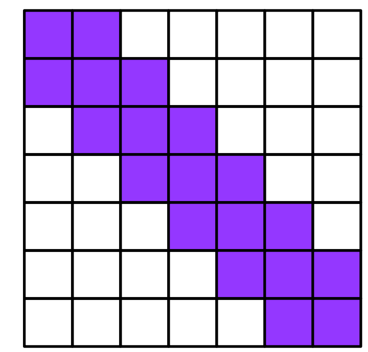

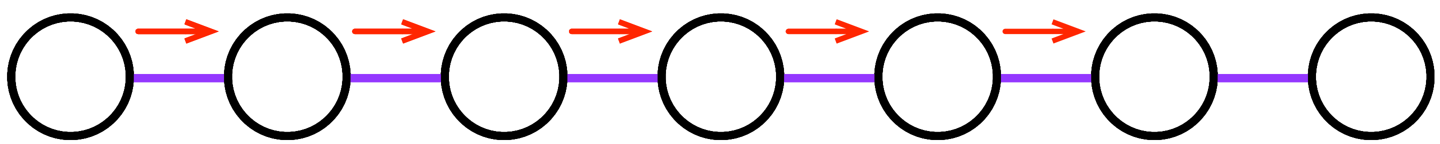

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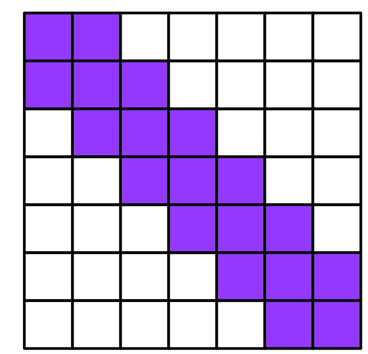
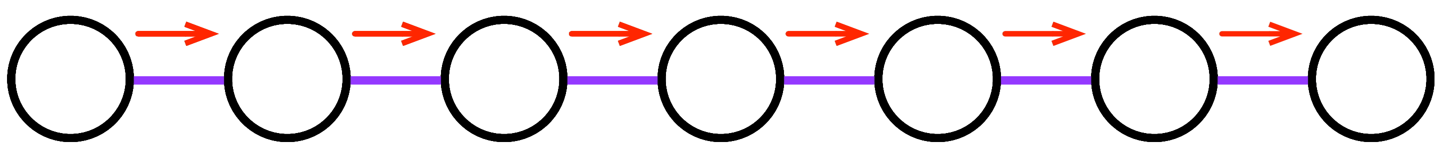
$\eta =$ 



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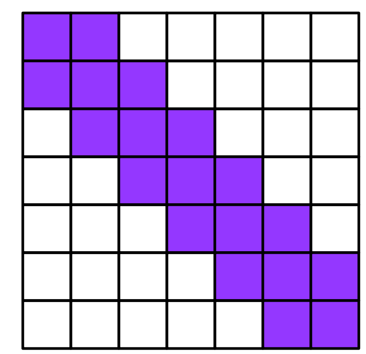

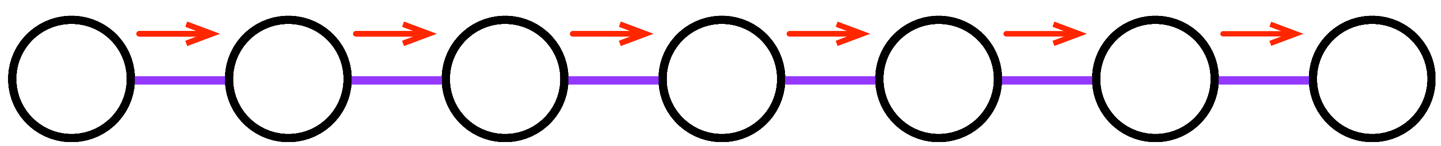

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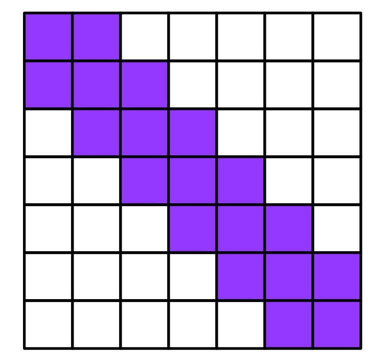
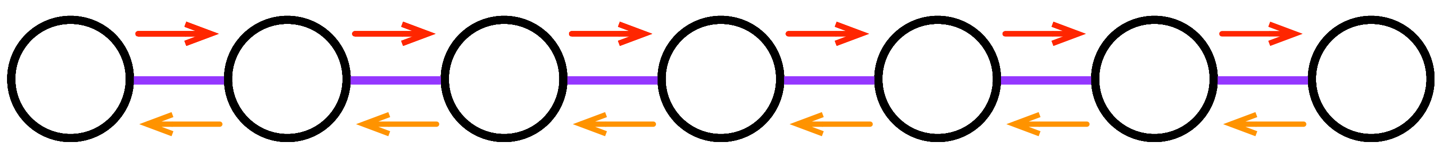
$\eta =$ 



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```
from scipy.stats import logsumexp

def log_normalizer(natparams, data):
  log_pi, log_A, log_B = natparams
  log_alpha = log_pi
  for y in data:
    log_alpha = logsumexp(log_alpha[:, None] + log_A, axis=0) + log_B[:, y]
  return logsumexp(log_alpha)


from autograd import grad
E_stats = grad(log_normalizer)(natparams, data)
```

https://github.com/HIPS/autograd/blob/master/examples/hmm_em.py

What about maximum likelihood?

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Say $\{x_n\}_{n=1}^N$ are samples, consider

$$\frac{1}{N}\log p(x\,;\,\eta) = \langle \eta,\ \frac{1}{N}\sum_{n=1}^{N} t(x_n)\rangle - \mathcal{A}(\eta)$$

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Claim

$$\nabla\mathcal{A}^*(\mu) = \arg\sup_{\eta\in\Theta} \langle \eta,\ \mu\rangle - \mathcal{A}(\eta)$$

$$\mathcal{A}^*(\mu) = \sup_{\eta \in \Theta} \langle \eta,\, \mu \rangle - \mathcal{A}(\eta) \qquad \mathcal{A}(\eta) = \sup_{\mu \in \mathcal{M}} \langle \eta,\, \mu \rangle - \mathcal{A}^*(\mu)$$

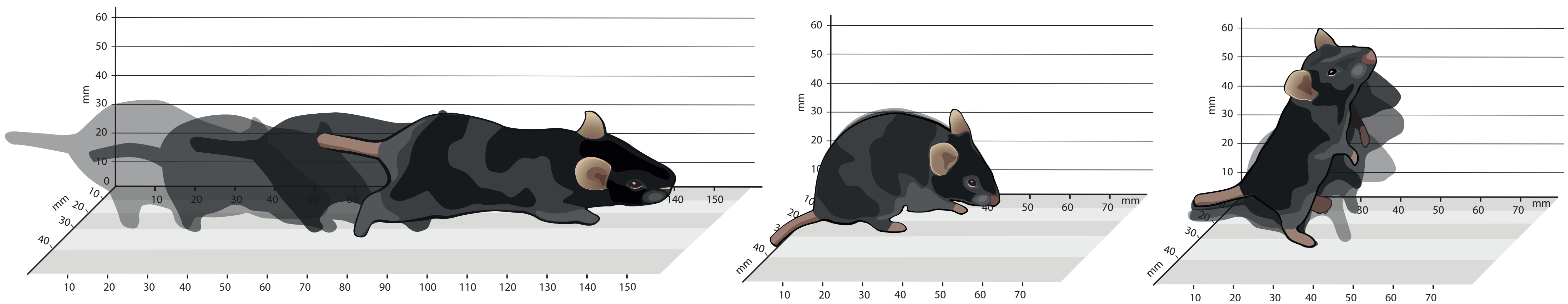
$$\eta(\mu) = \nabla \mathcal{A}^*(\mu) \qquad \mu(\eta) = \nabla \mathcal{A}(\eta)$$

Summary for tractable exponential families

For each tractable exponential family…

1. implement $t(x)$ and $\mathcal{A}(\eta)$ for exact inference
   and mean field variational inference
2. implement $\mathcal{A}^*(\mu)$ for maximum likelihood
   and (variational) expectation-maximization (EM)
3. implement `sample` for drawing samples
   and Gibbs sampling MCMC

Next up: composing tractable families into intractable ones!


mm
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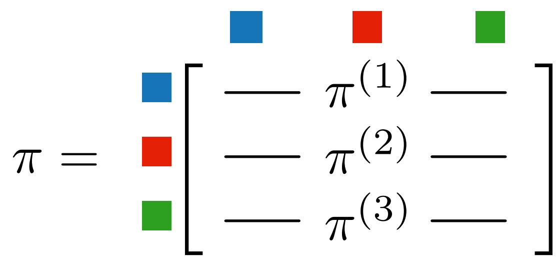
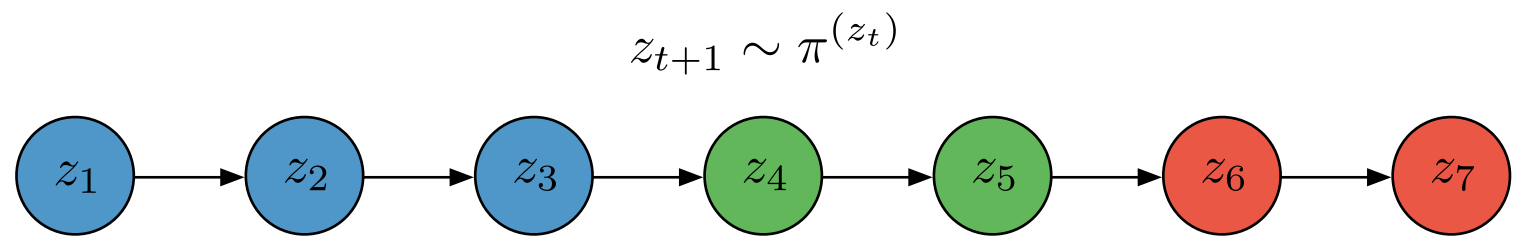
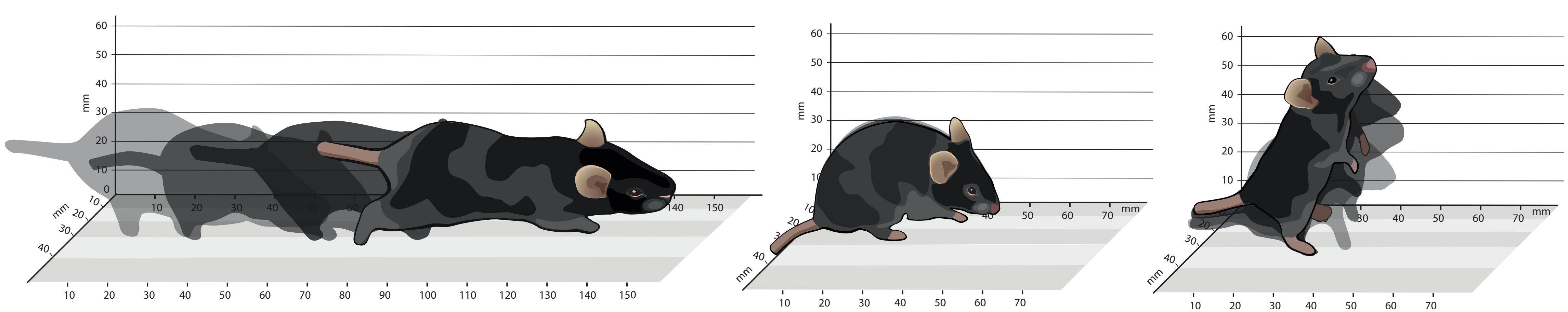
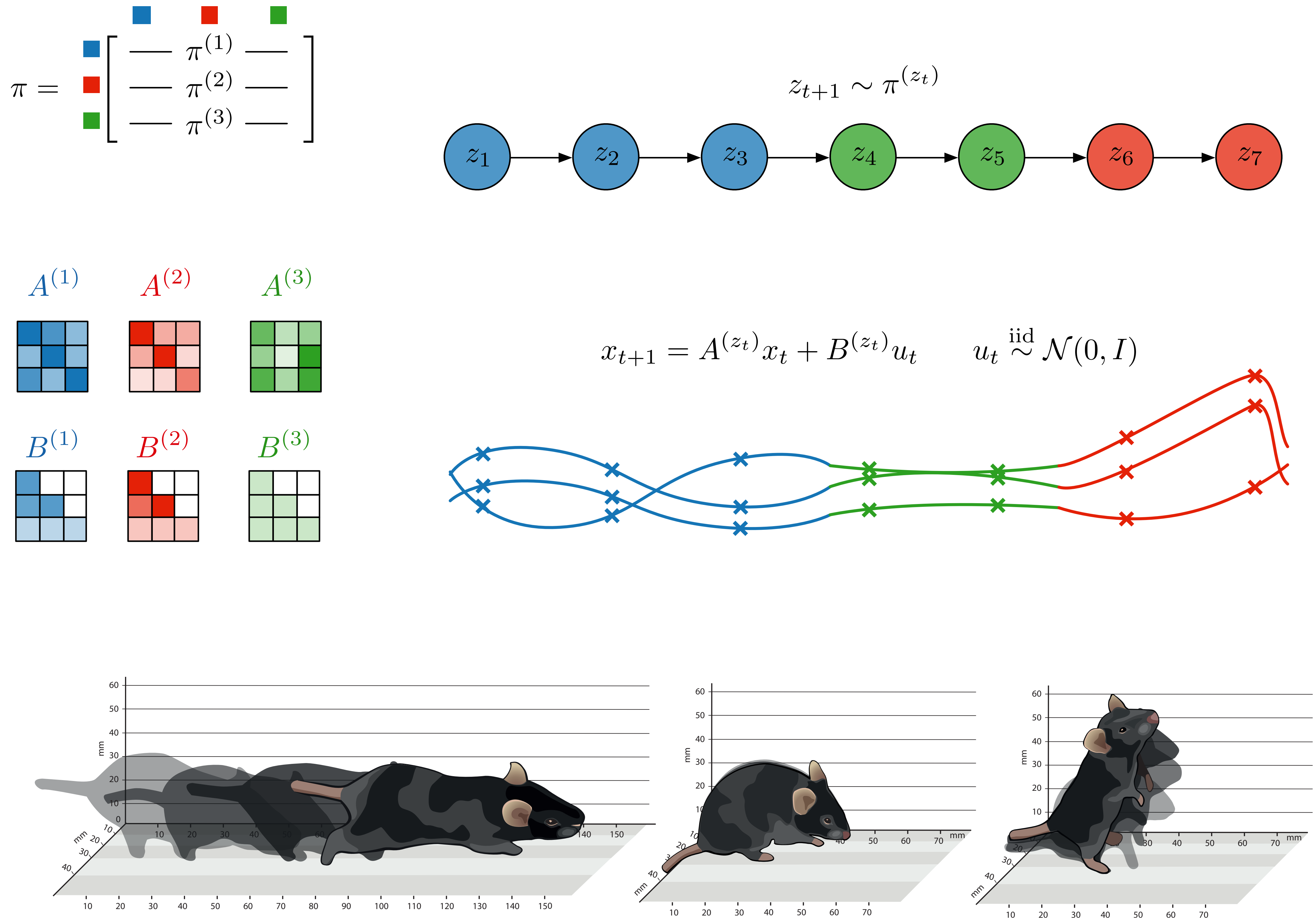

$\pi = \begin{bmatrix} — \pi^{(1)} — \\ — \pi^{(2)} — \\ — \pi^{(3)} — \end{bmatrix}$


$z_{t+1} \sim \pi^{(z_t)}$
z_1 z_2 z_3 z_4 z_5 z_6 z_7





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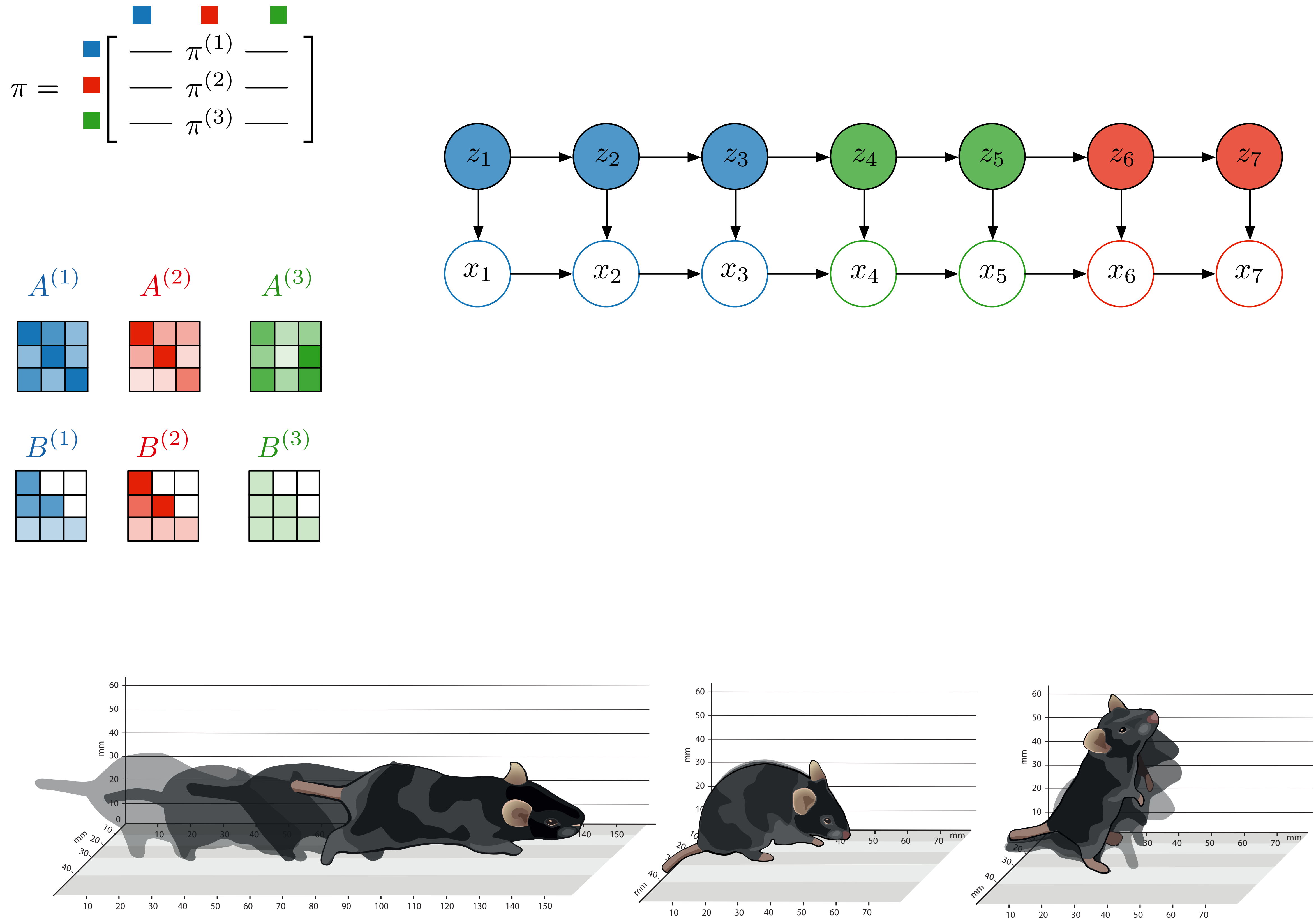
z_1 z_2 z_3 z_4 z_5 z_6 z_7
$A^{(1)}$ $A^{(2)}$ $A^{(3)}$
$B^{(1)}$ $B^{(2)}$ $B^{(3)}$
$x_{t+1} = A^{(z_t)} x_t + B^{(z_t)} u_t \qquad u_t \overset{\text{iid}}{\sim} \mathcal{N}(0, I)$
mm



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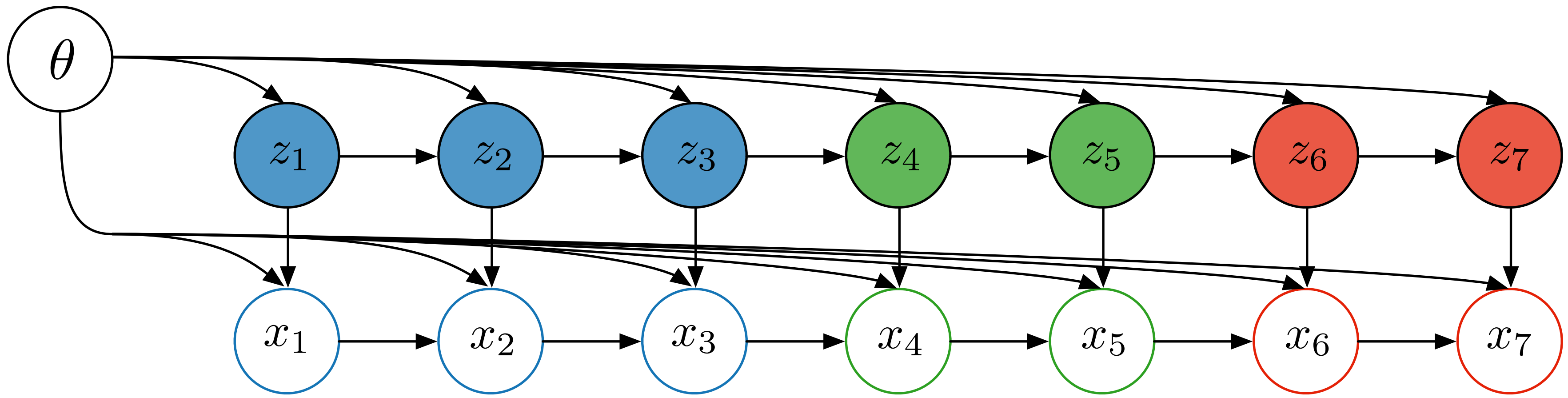

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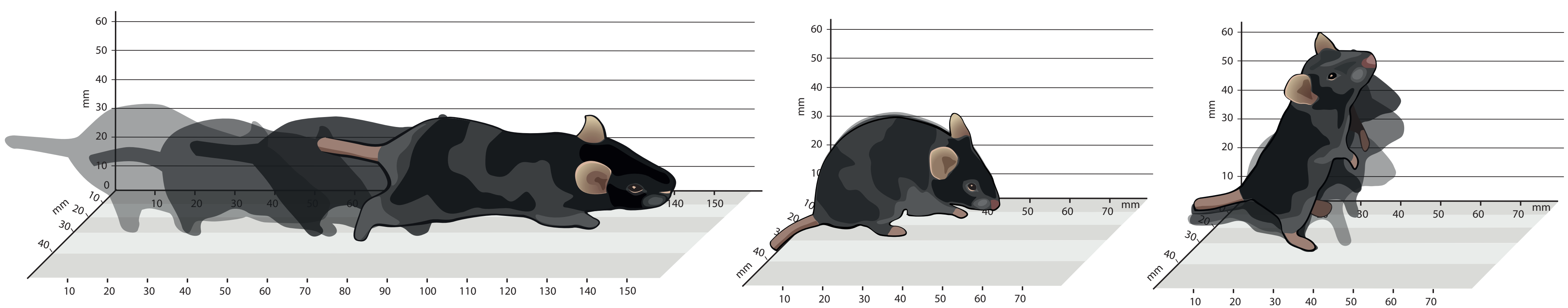

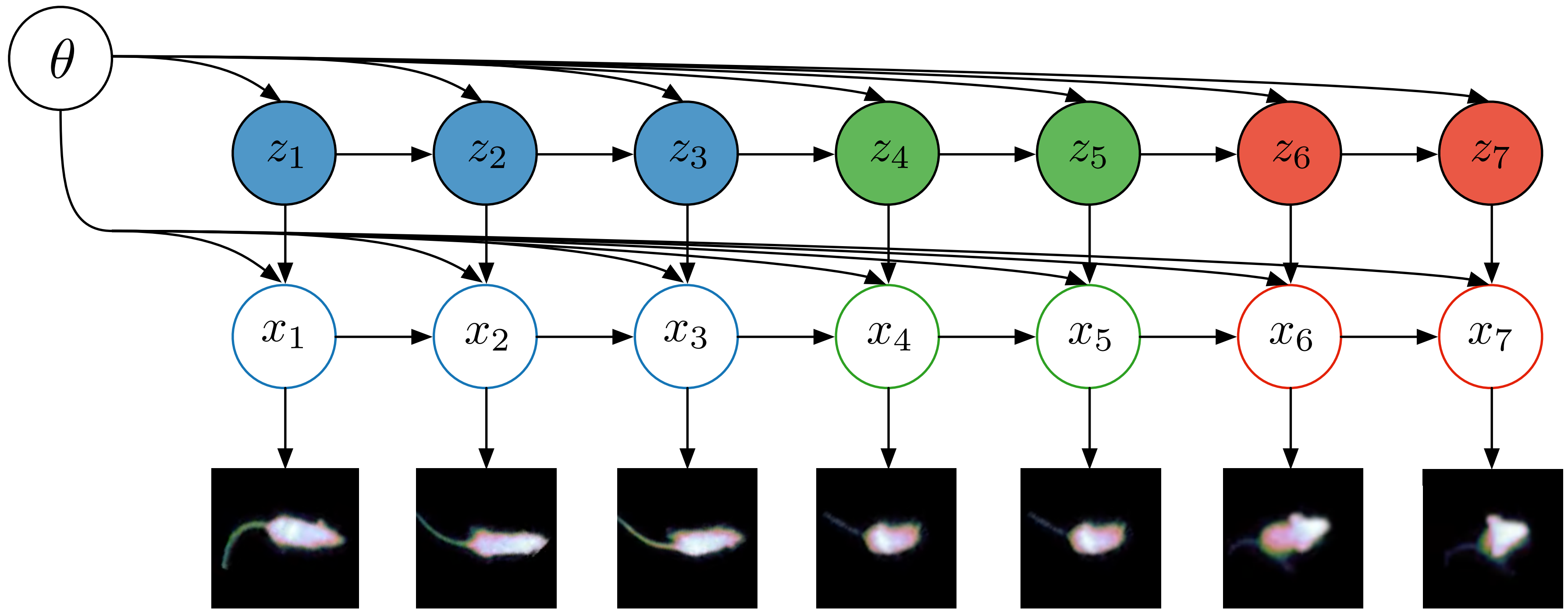
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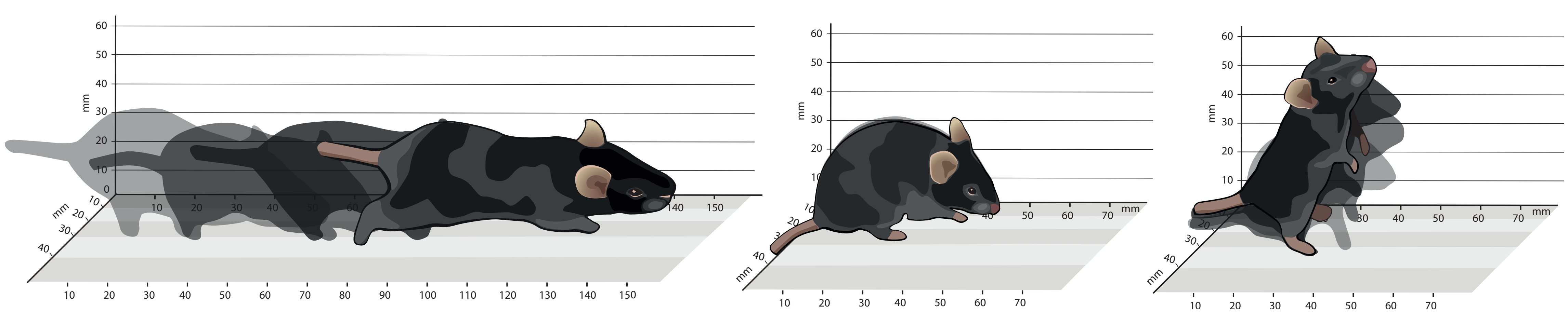
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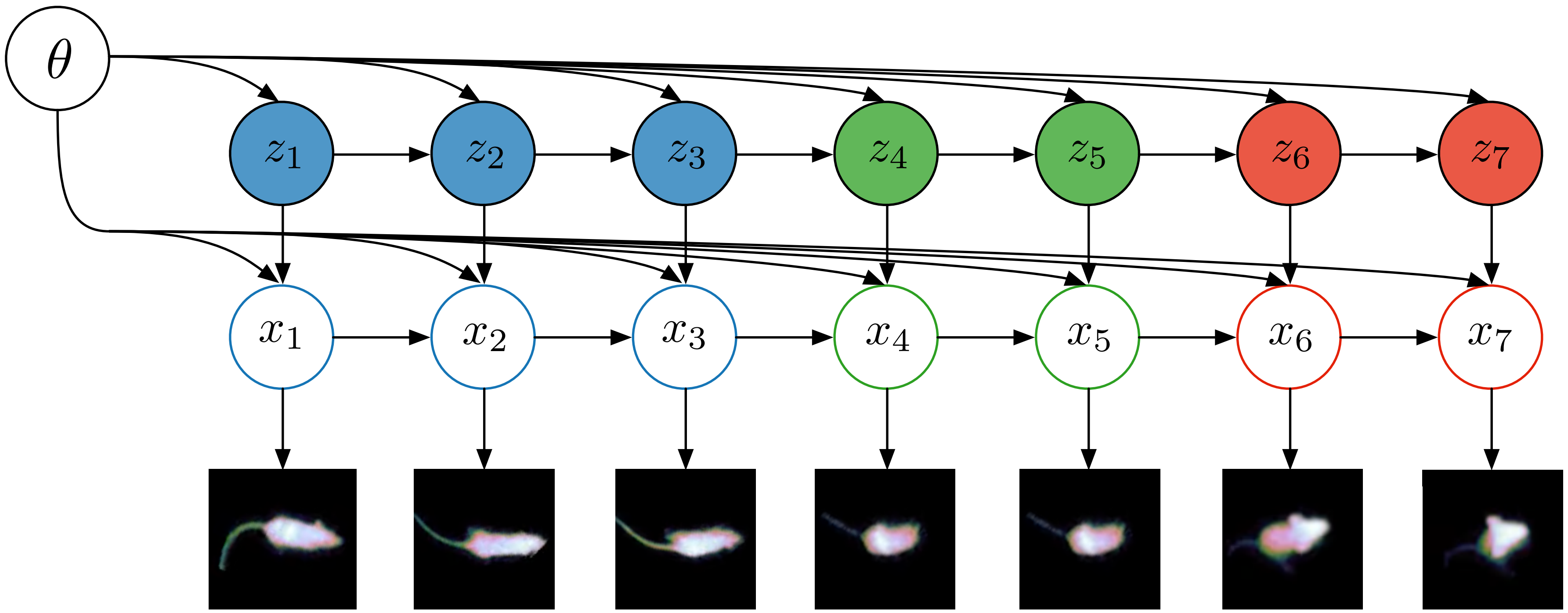

θ
z_1
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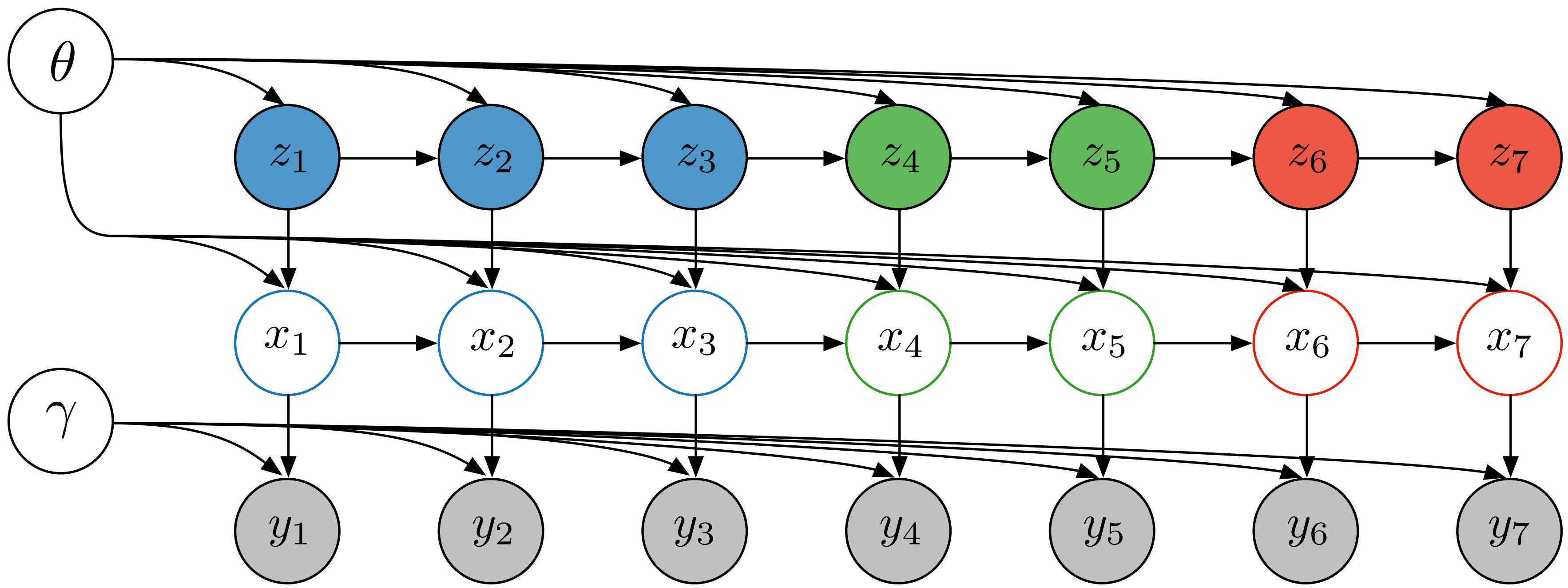

$$y_t \mid x_t \sim \mathcal{N}(Cx_t, \Sigma), \qquad \gamma = (C, \Sigma)$$

Compose exp. families, get compositional algorithms?

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For $x = (x_1, x_2)$ consider a negative energy function

$$\begin{aligned}\log p(x\,;\,\eta) &= \langle \eta,\ t(x)\rangle + \text{const.}\\ &= \langle \eta_{10},\ t_1(x_1)\rangle + \langle \eta_{01},\ t_2(x_2)\rangle\\ &\quad + \langle \eta_{11},\ t_1(x_1) \otimes t_2(x_2)\rangle + \text{const.}\end{aligned}$$

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$$\log p(x_1 \mid x_2) = \langle \eta_{10} + \eta_{11} \cdot t_2(x_2),\, t_1(x_1) \rangle + \text{const.}$$

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But the normalizer $\mathcal{A}$ is not tractable!

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Can we build algorithms for

1. approximate sampling $x \sim p(x\,;\,\eta)$ via MCMC?
2. approximate expectations $\mathbb{E}[t(X)]$ and $\mathcal{A}$?
3. variational Expectation-Maximization to estimate η?

that exploit the tractable parts?

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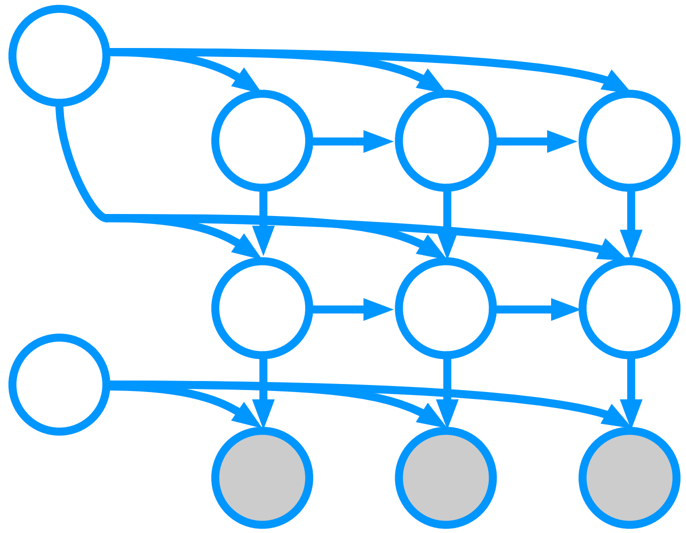

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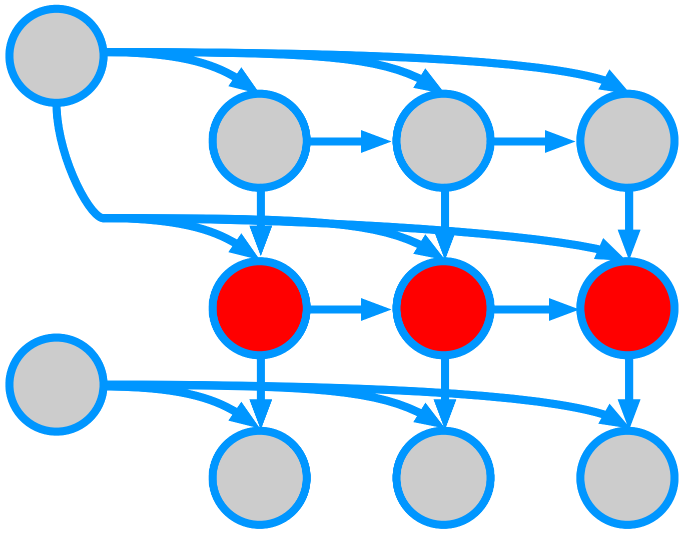

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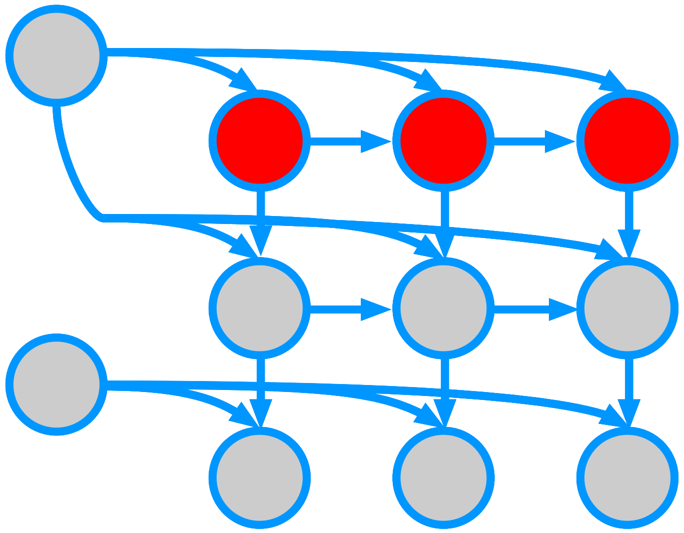

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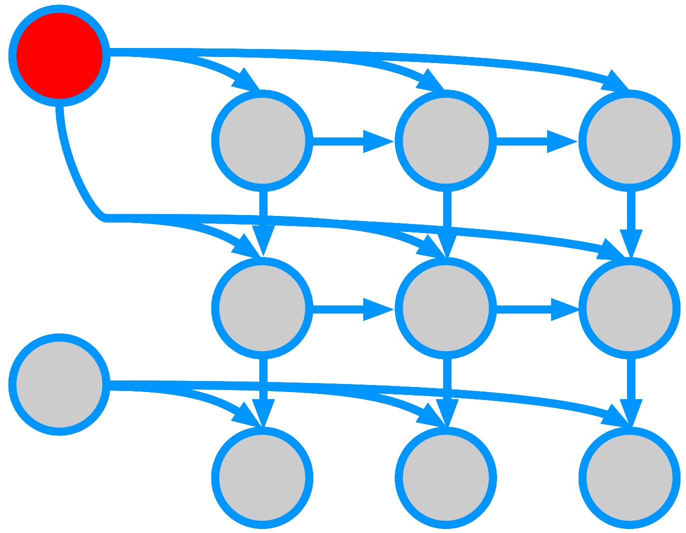

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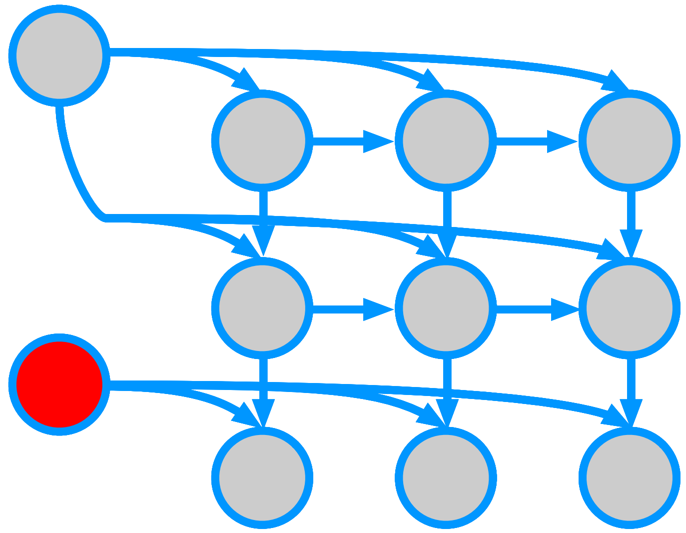

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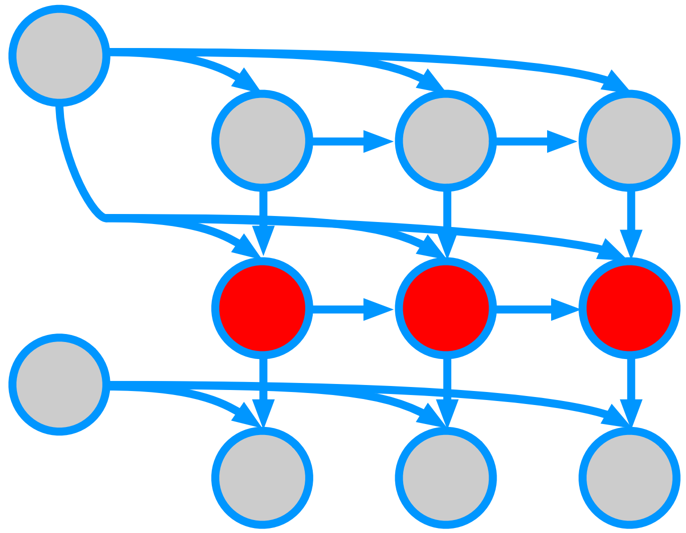

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Claim [Gibbs sampling]

$$p(x_m \,|\, x_{\neg m}) = \exp(\langle \eta_m^*, t_m(x_m) \rangle - \mathcal{A}_m(\eta_m^*))$$

$$\eta_m^* \triangleq \nabla_m g(t_1(x_1), \ldots, t_M(x_M))$$

```
from autograd import grad

def gibbs(g, samplers, niter, x):
  for _ in range(niter):
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```

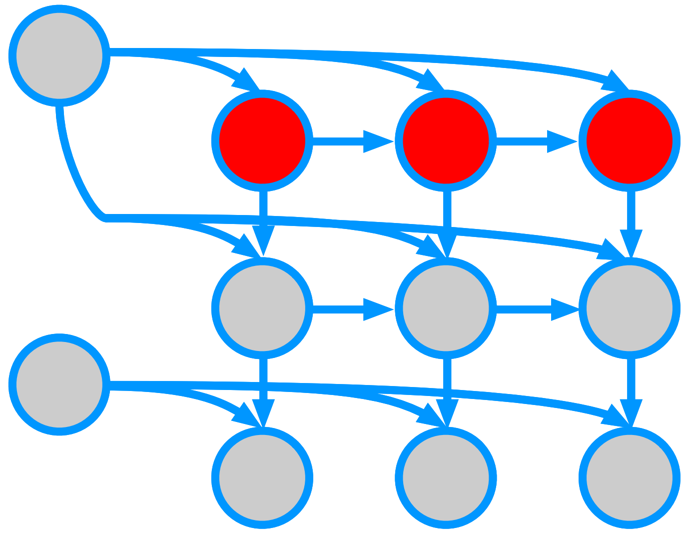

$$\log p(x\,;\,\eta) = \langle \eta,\, t(x) \rangle + \text{const.}$$

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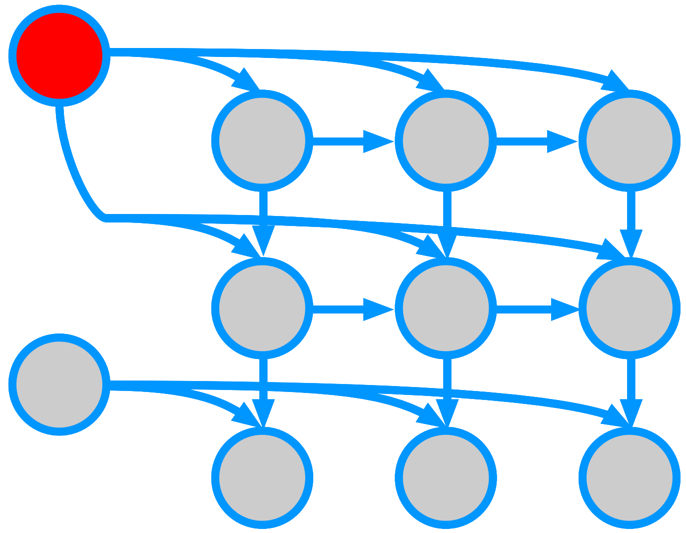

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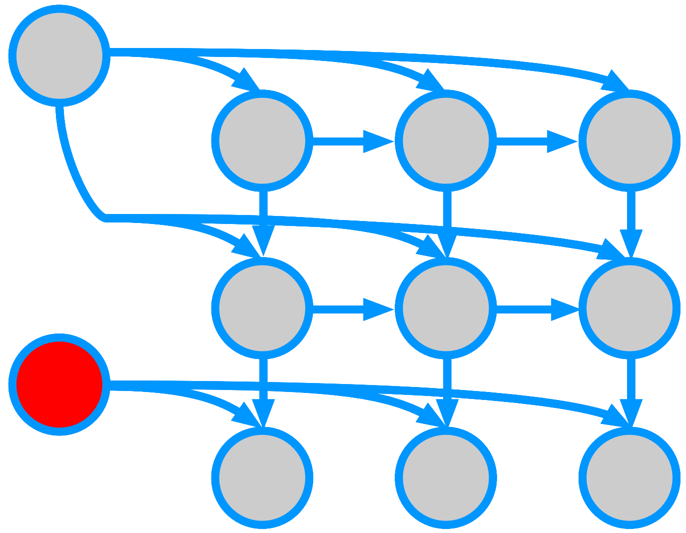

Consider the variational family

$$q(x) = \prod_{m=1}^{M} q_m(x_m\,;\,\eta_m)$$

$$q(x_m\,;\,\eta_m) = \exp(\langle \eta_m, t_m(x_m)\rangle - \mathcal{A}_m(\eta_m))$$

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Claim [Variational lower bound]

$$\mathcal{A}(\eta) \geq \langle \eta,\, \mathbb{E}_q[t(X)]\rangle - \sum_m \mathcal{A}_m^*(\mu_m)$$

$$= g(\mu_1, \ldots, \mu_M) - \sum_m \mathcal{A}_m^*(\mu_m) \triangleq \mathcal{L}(\eta)$$

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Claim [Variational lower bound]

$$\begin{aligned}\mathcal{A}(\eta) &\geq \langle \eta,\, \mathbb{E}_q[t(X)] \rangle - \textstyle\sum_m \mathcal{A}_m^*(\mu_m) \\ &= g(\mu_1, \ldots, \mu_M) - \textstyle\sum_m \mathcal{A}_m^*(\mu_m) \triangleq \mathcal{L}(\eta)\end{aligned}$$

Proof Use the variational definition of $\mathcal{A}$:

$$\mathcal{A}(\eta) = \sup_{\mu \in \mathcal{M}} \langle \eta,\, \mu \rangle - \mathcal{A}^*(\mu)$$

Consider the variational family

$$q(x) = \prod_{m=1}^{M} q_m(x_m\,;\,\eta_m)$$

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$$g(\nabla \mathcal{A}_1(\eta_1), \ldots, \nabla \mathcal{A}_M(\eta_M)) - (\textstyle\sum_m \langle \eta_m,\, \nabla \mathcal{A}_m(\eta_m) \rangle - \mathcal{A}_m(\eta_m))$$

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Claim [Structured mean field]

$$\arg\max_{\eta_m} \mathcal{L}(\eta_1, \ldots, \eta_M) = \nabla_m g(\mu_1, \ldots, \mu_M))$$

$$\text{where} \;\; \mu_{m'} = \nabla \mathcal{A}_{m'}(\eta_{m'}) \;\; \text{for} \;\; m' = 1, \ldots, M$$

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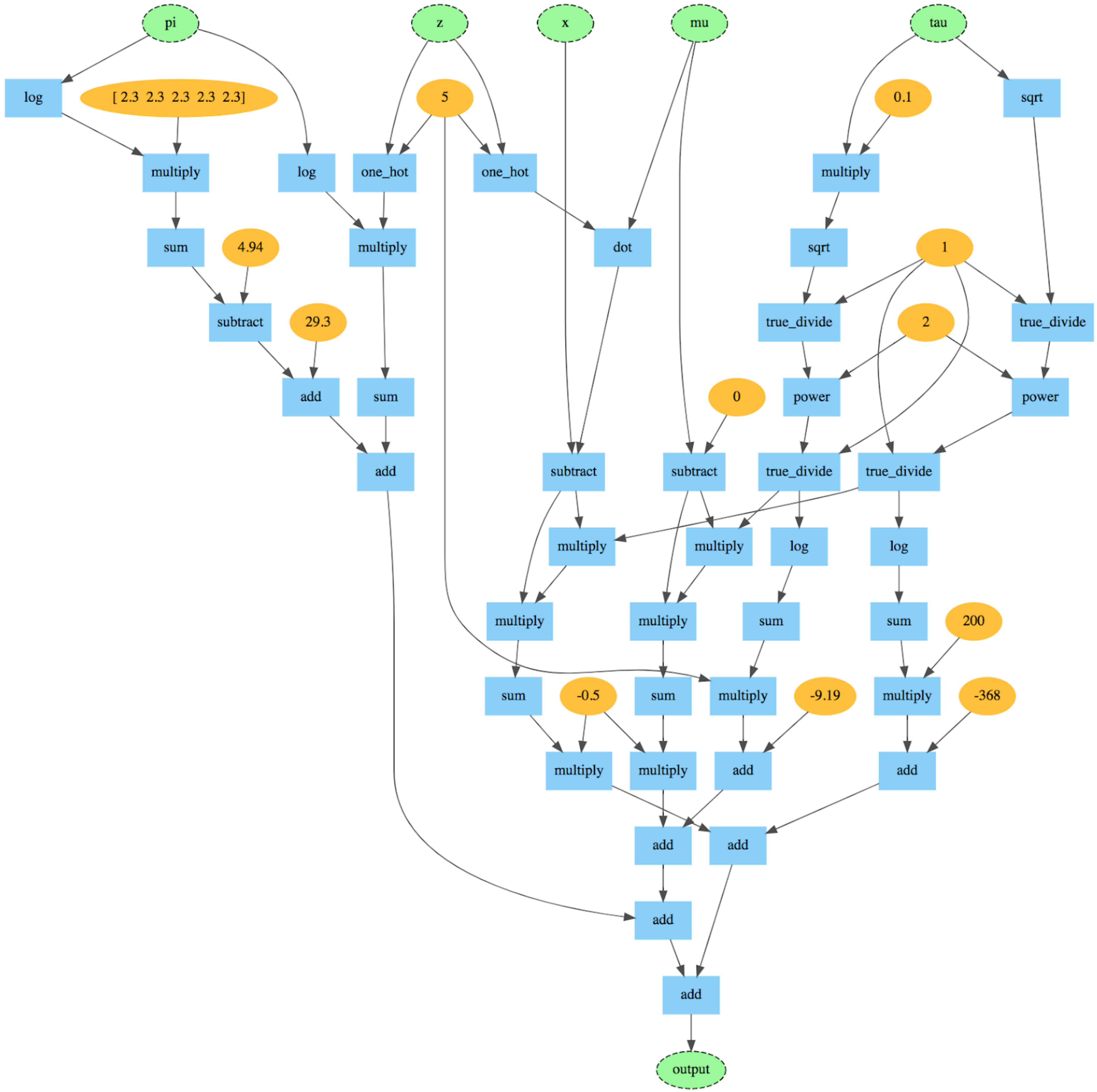
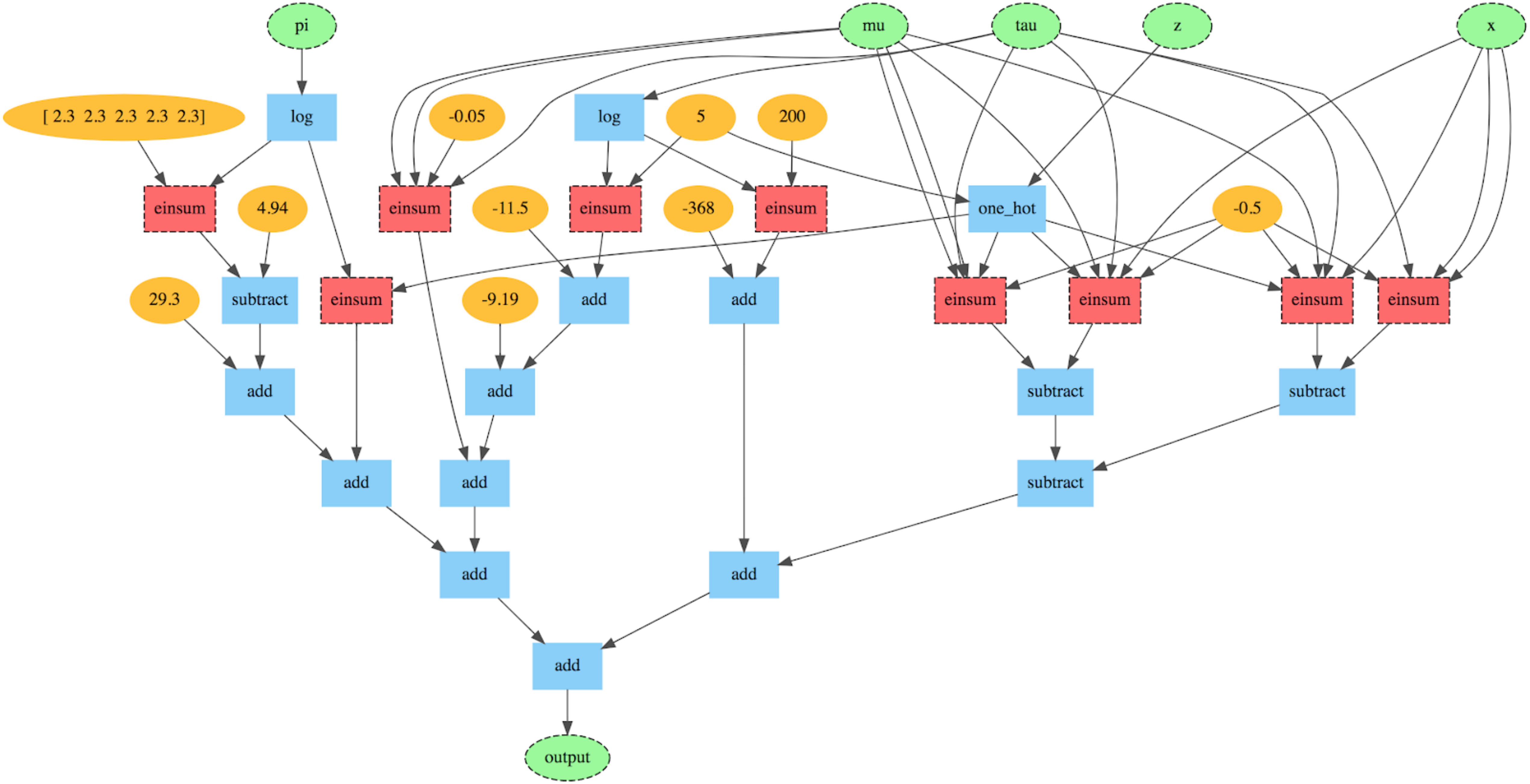
```
def meanfield(g, As, etas):
  def meanfield_sweep(mus):
    for m in range(M):
      mus[m] = grad(As[m])(grad(g, m)(*mus))
    return mus

  mus = [grad(As[m])(etas[m]) for m in range(M)]
  mu_stars = fixed_point(meanfield_sweep, mus)
  return [grad(g, m)(*mu_stars) for m in range(M)]
```

```python
def neg_energy(eta_prior, t_y, t_theta, t_z, t_x):
  t_z_node = markovchain.pair_to_node(t_z)
  t_z_trans = t_z[..., :-1, :, :]
  t_x_init = lds.pair_to_node(t_x[..., 0, :, :])
  t_x_trans = t_x[..., :-1, :, :]
  t_xy = gaussian.stats_product(lds.pair_to_node(t_x), t_y)
  return dot(eta_prior, t_theta) - logZ_theta(eta_prior)                  \
      + np.einsum('i,...i->',        t_theta[0], t_z_node[..., 0, :])       \
      + np.einsum('ij,...tij->',     t_theta[1], t_z_trans)                 \
      + np.einsum('kij,k,...ij->',   t_theta[2], t_z_node[..., 0, :], t_x_init)  \
      + np.einsum('kij,tk,...tij->', t_theta[3], t_z_node, t_x)             \
      + np.einsum('ij,...tij->',     t_theta[4], t_xy)
```

```python
def normal_logpdf(x, loc,  scale):
  prec = 1. / scale**2
  return -(np.sum(prec * mu**2) - np.sum(np.log(prec))
           + np.log(2. * np.pi)) * N / 2.

def normal_logpdf(pi, z, mu, tau, x):
  logp = (np.sum((alpha-1) * np.log(x)) - np.sum(gammaln(alpha))
          + np.sum(gammaln(np.sum(alpha, -1))))
  logp += normal_logpdf(mu, 0., 1./np.sqrt(kappa * tau))
  logp += np.sum(one_hot(z, K) * np.log(pi))
  logp += (a-1)*np.log(tau) - b*tau + a*np.log(b) - gammaln(a)
  mu_z = np.dot(one_hot(z, K), mu)
  loglike = normal_logpdf(x, mu_z, 1./np.sqrt(tau))
  return logp + loglike
```


pi
z
x
mu
tau
log
[2.3 2.3 2.3 2.3 2.3]
5
sqrt
0.1
multiply
log
one_hot
one_hot
multiply
sum
4.94
multiply
dot
sqrt
1
subtract
29.3
true_divide
2
true_divide
add
sum
0
power
power
add
subtract
subtract
true_divide
true_divide
multiply
multiply
log
log
multiply
multiply
sum
sum
200
sum
-0.5
sum
multiply
-9.19
multiply
-368
multiply
multiply
add
add
add
add
add
add
output



pi
mu
tau
z
x
[2.3 2.3 2.3 2.3 2.3]
log
-0.05
log
5
200
einsum
4.94
einsum
-11.5
einsum
-368
einsum
one_hot
-0.5
29.3
subtract
einsum
-9.19
add
add
einsum
einsum
einsum
einsum
add
add
subtract
subtract
add
add
subtract
add
add
add
output

Domain-specific term graph rewriting implementation

- **Tracer** using Autograd's API to map Python to term graphs
- **Pattern matcher** to do pattern-directed invocation
    - Python-embedded pattern language
    - Compiled into **continuation-passing matcher combinators** (~300 loc)

```
pat = (Einsum, Str('formula'), Segment('args1'),
       (Choice(Subtract('op'), Add('op')), Val('x'), Val('y')), Segment('args2'))
```

- **Rewriters** are syntactic graph macros using tracing to get **quasi-quasiquotes**

```
def rewriter(formula, op, x, y, args1, args2):
  return op(np.einsum(formula, *(args1 + (x,) + args2)),
            np.einsum(formula, *(args1 + (y,) + args2)))

distribute_einsum = Rule(pat, rewriter) # Rule is a namedtuple
```

Goals

1. Motivate why PGMs + DNNs are a revolution waiting to happen
2. Survey the fundamentals of PGMs and exponential families so that you have a broad view of the territory
3. Show how to unify many models and algorithms in a framework that lets you leverage automatic differentiation
4. Make SVAEs and related PGM + DNN architectures super obvious so that you can invent better ones

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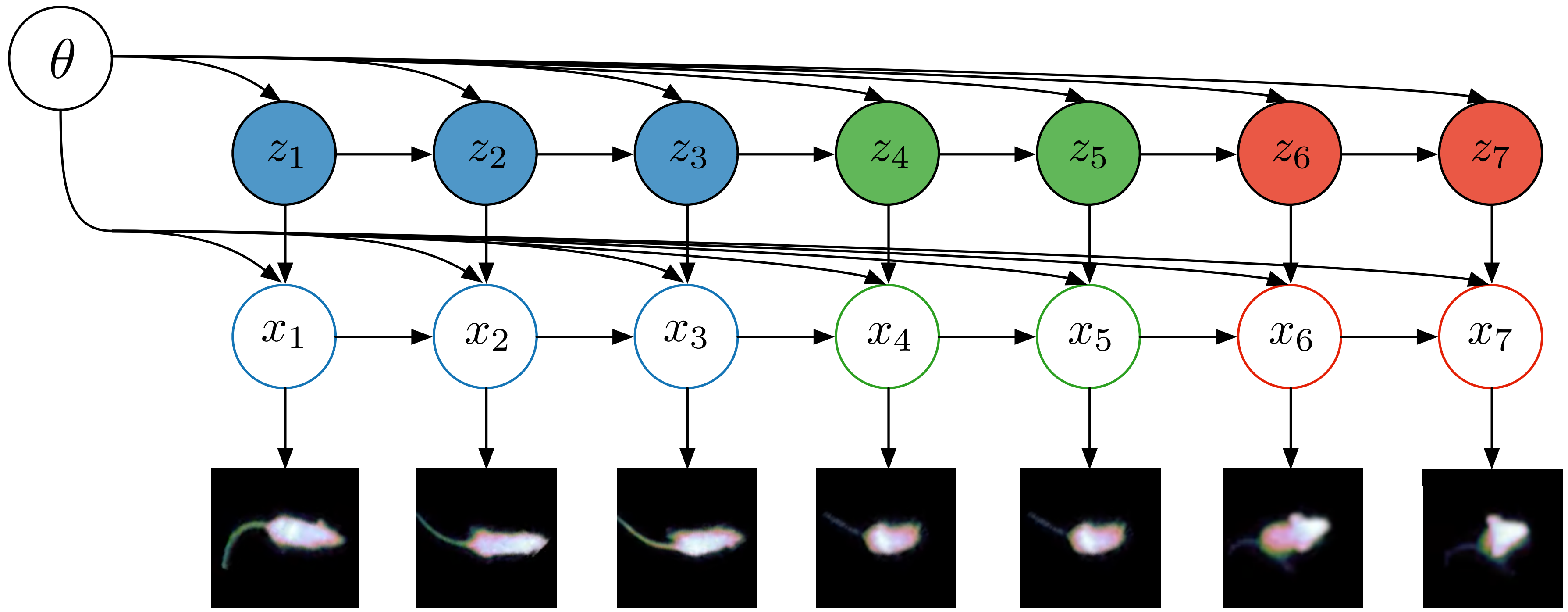
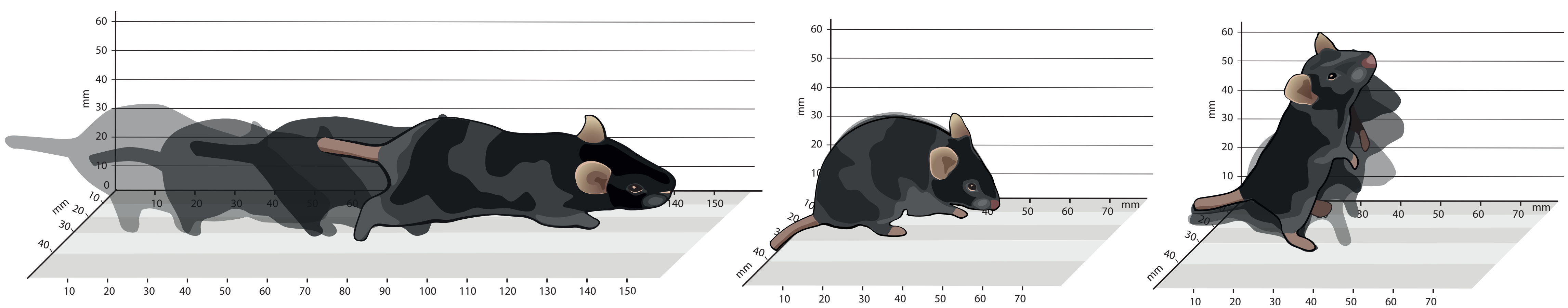
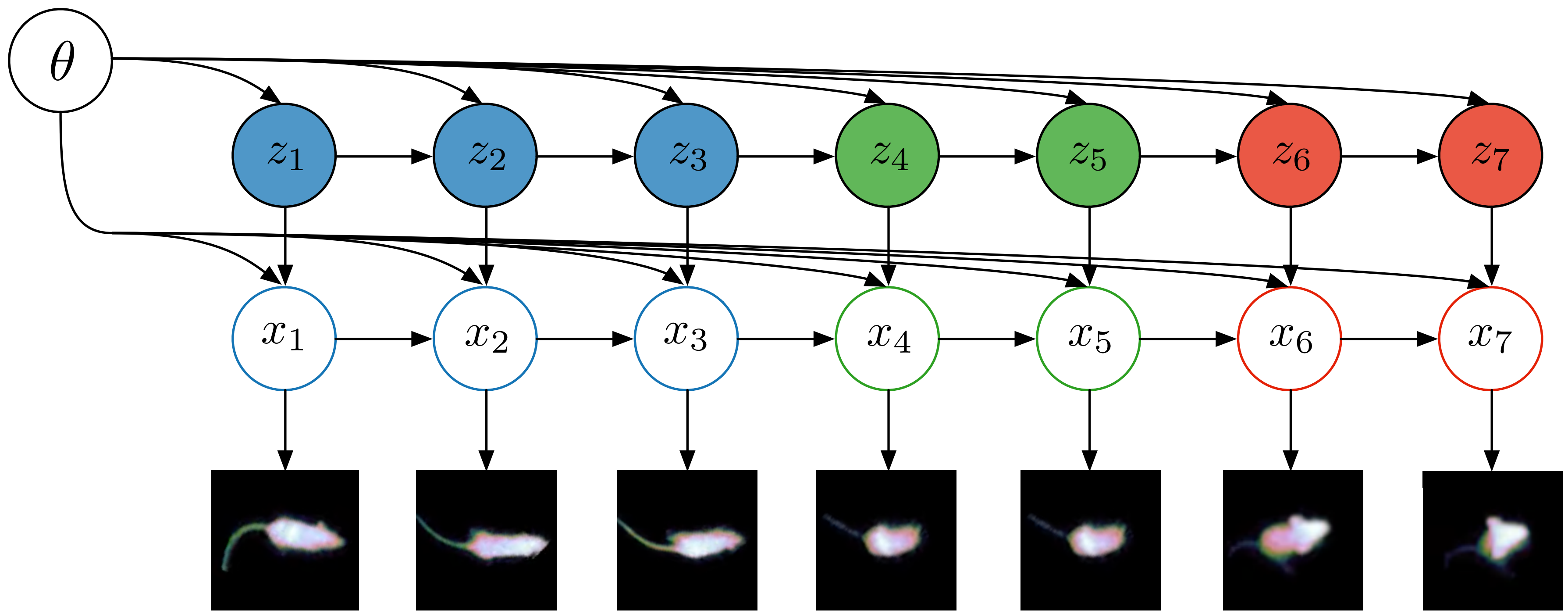


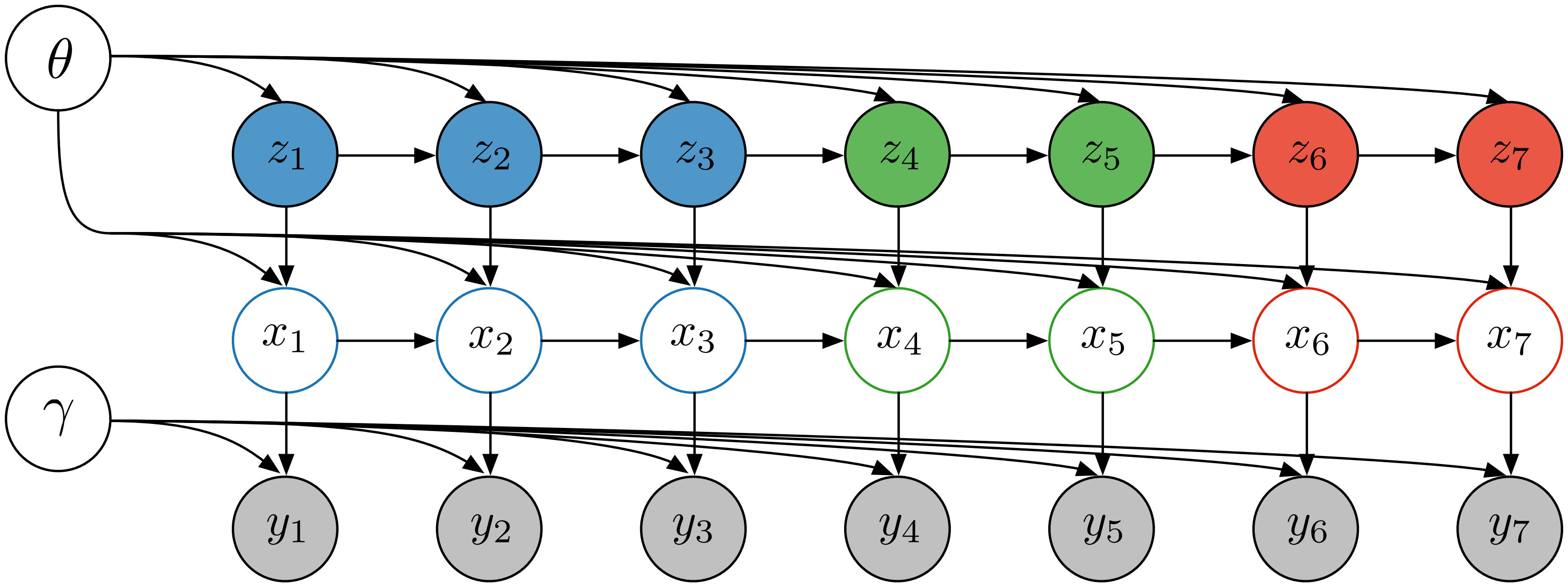
θ
z_1
z_2
z_3
z_4
z_5
z_6
z_7
x_1
x_2
x_3
x_4
x_5
x_6
x_7



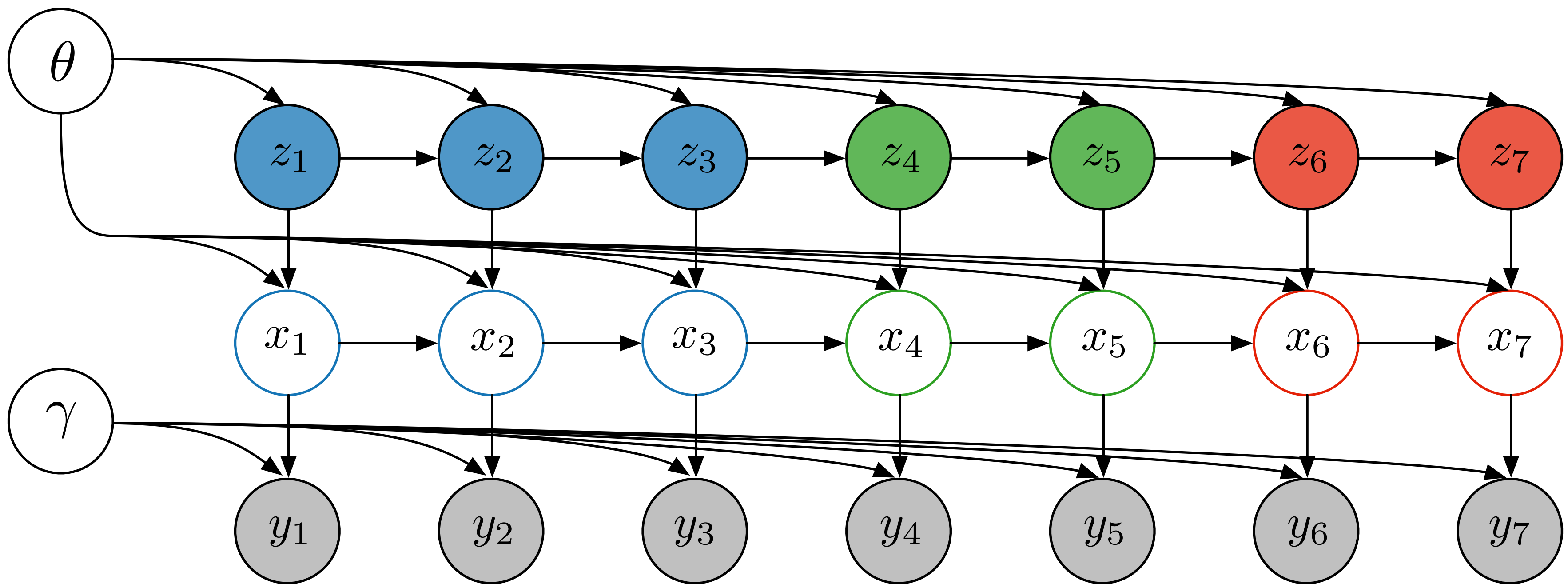
mm



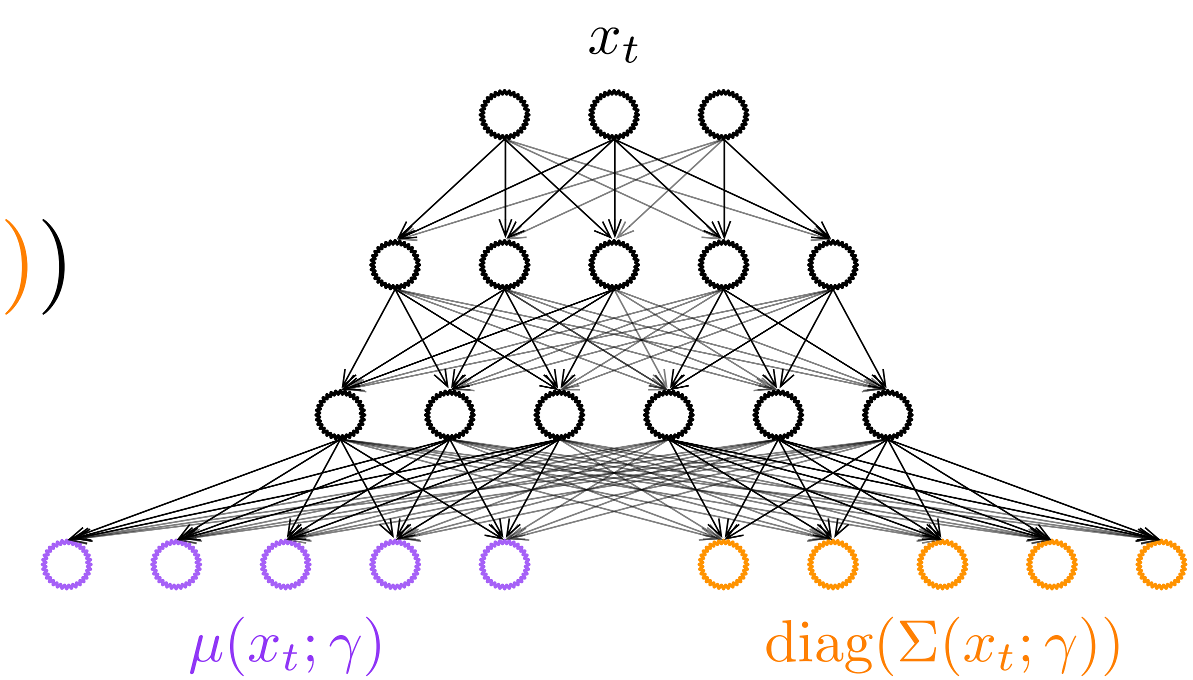
θ
z_1
z_2
z_3
z_4
z_5
z_6
z_7
x_1
x_2
x_3
x_4
x_5
x_6
x_7

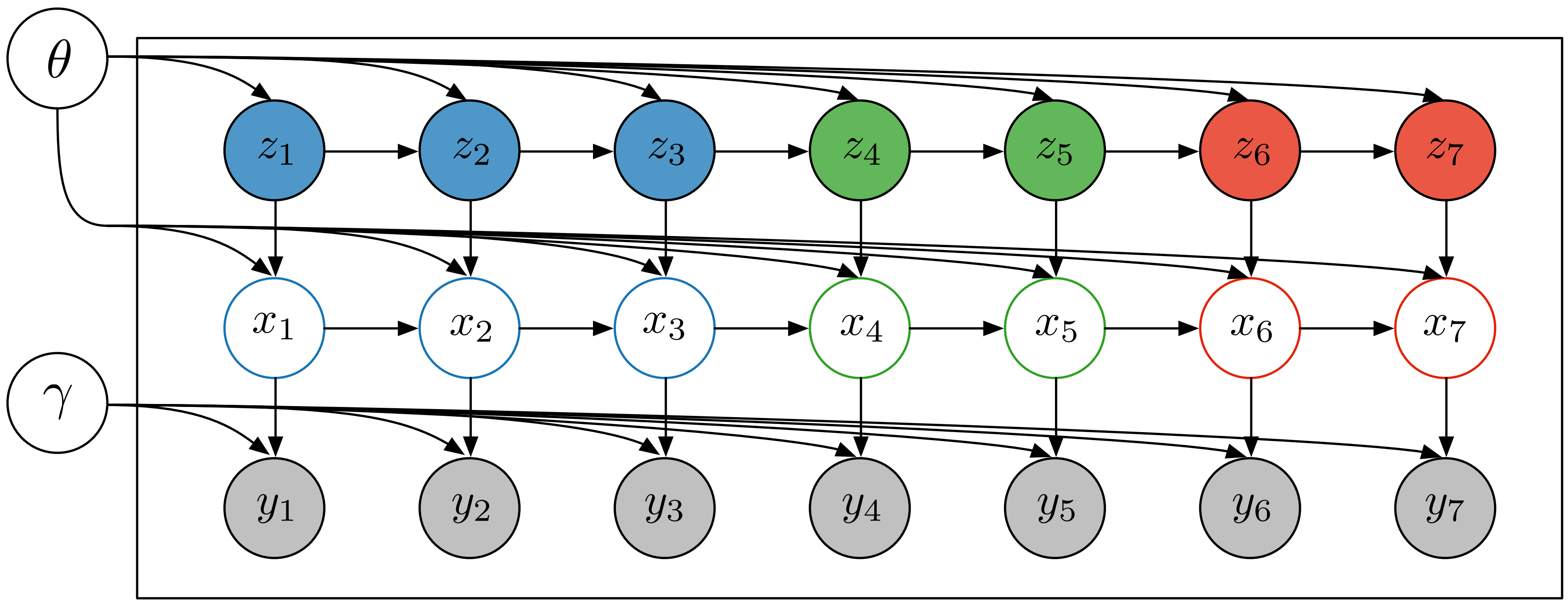


θ
z_1
z_2
z_3
z_4
z_5
z_6
z_7
x_1
x_2
x_3
x_4
x_5
x_6
x_7
γ
y_1
y_2
y_3
y_4
y_5
y_6
y_7



$$y_t \mid x_t, \gamma \;\sim\; \mathcal{N}(\mu(x_t;\gamma), \Sigma(x_t;\gamma))$$





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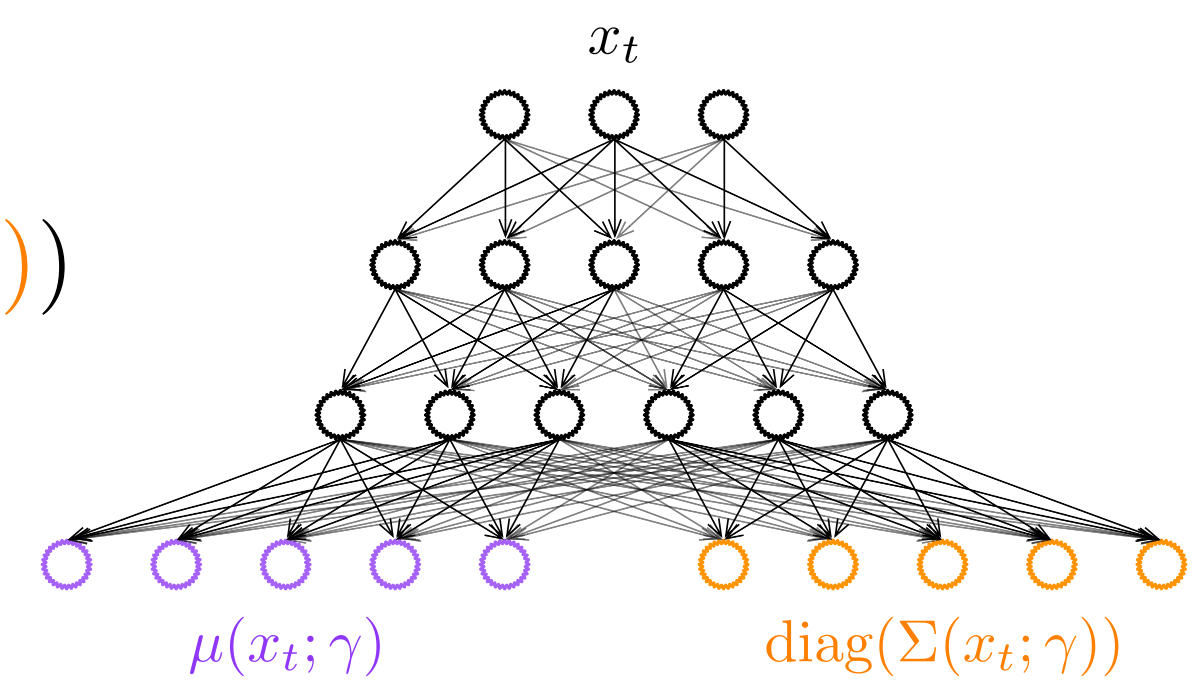
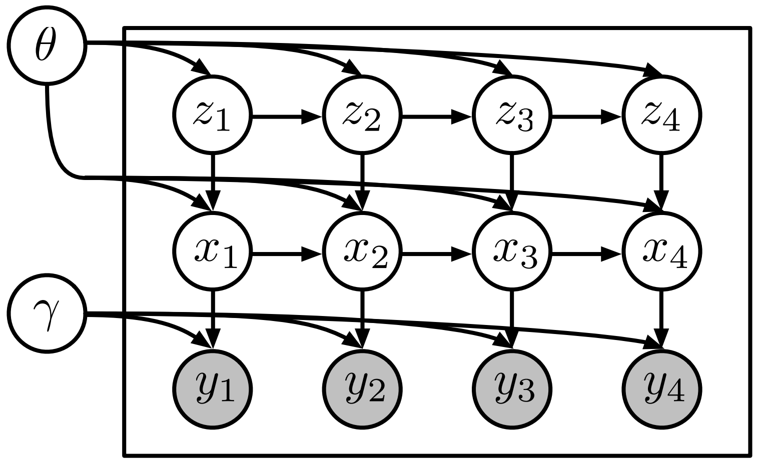
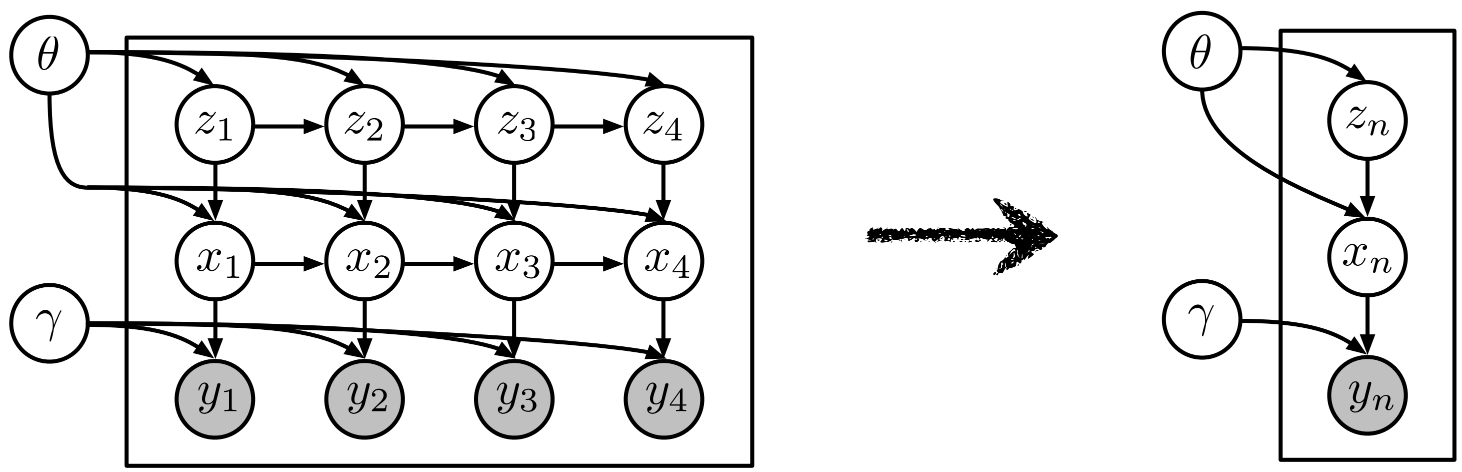
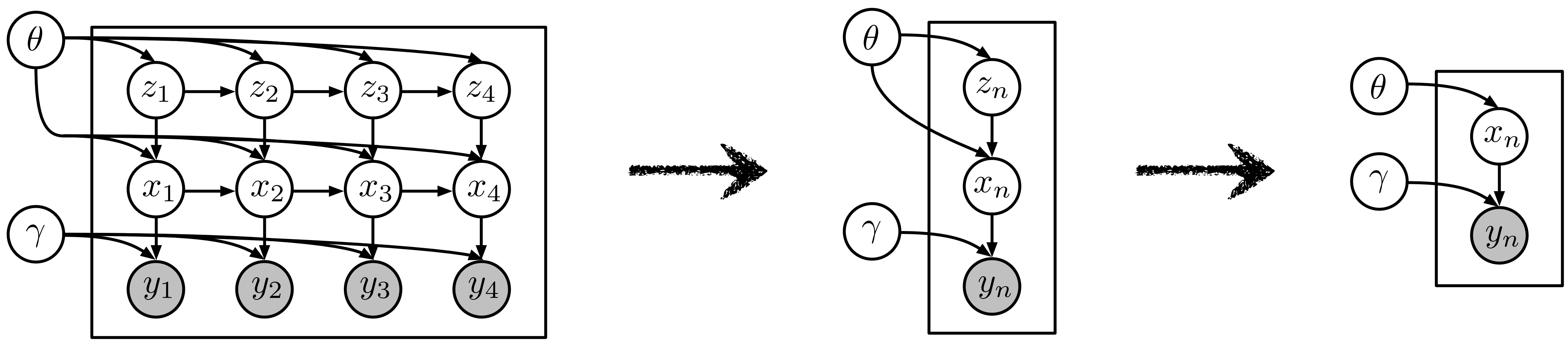


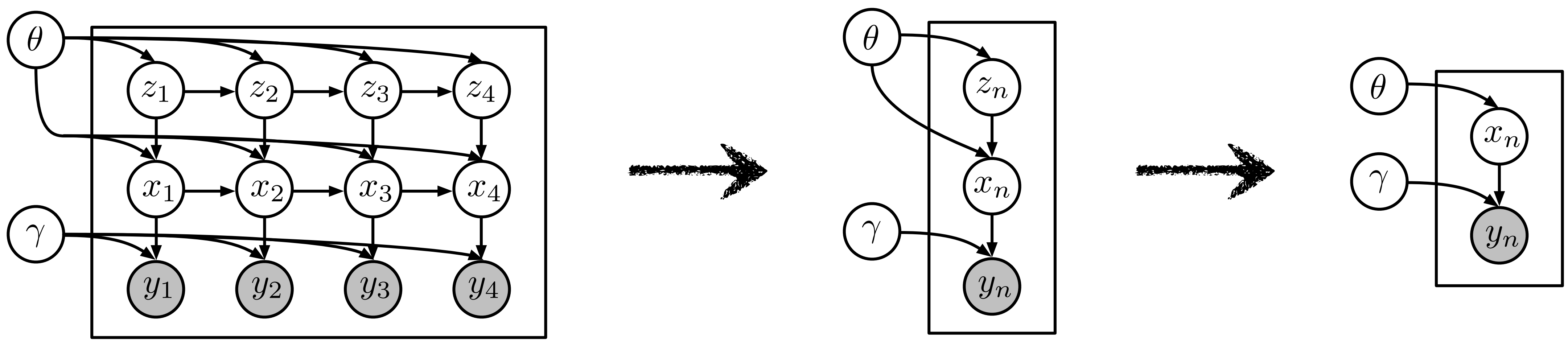


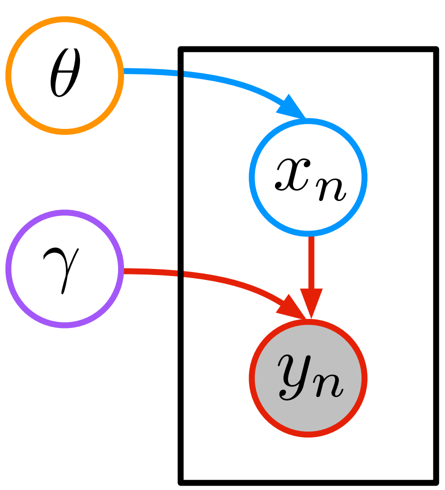
θ
z_1
z_2
z_3
z_4
x_1
x_2
x_3
x_4
γ
y_1
y_2
y_3
y_4

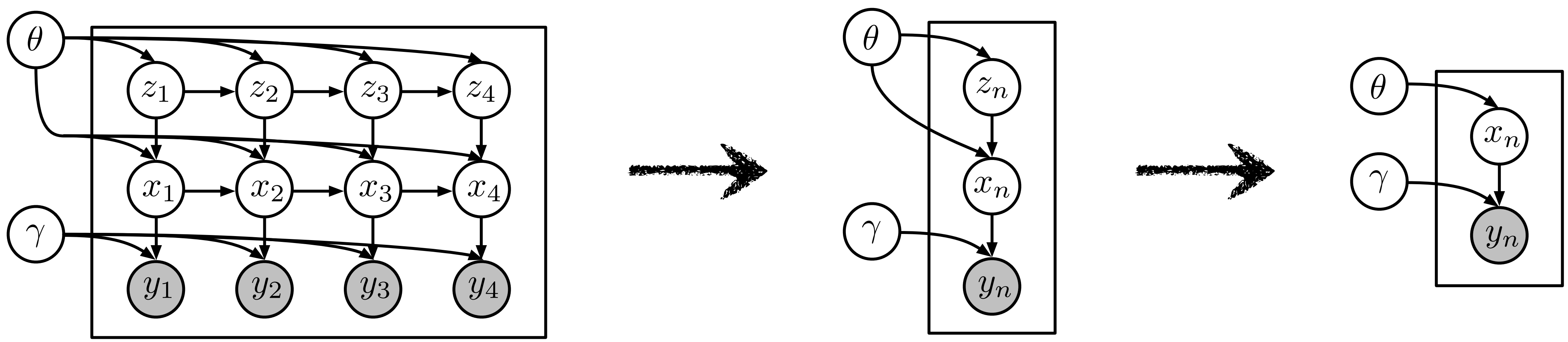

θ
z_1
z_2
z_3
z_4
x_1
x_2
x_3
x_4
γ
y_1
y_2
y_3
y_4
θ
z_n
x_n
γ
y_n

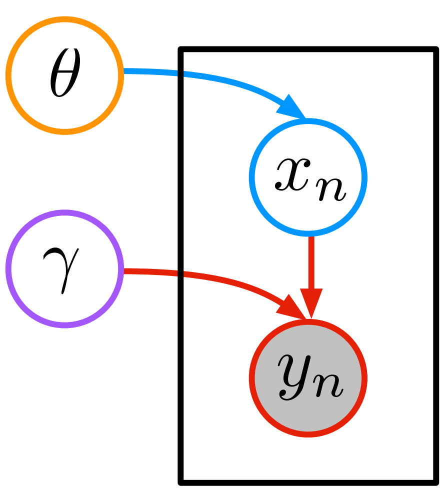


θ
γ
z_1 z_2 z_3 z_4
x_1 x_2 x_3 x_4
y_1 y_2 y_3 y_4
θ
γ
z_n
x_n
y_n
θ
γ
x_n
y_n


θ
γ
z1 z2 z3 z4
x1 x2 x3 x4
y1 y2 y3 y4
zn
xn
yn

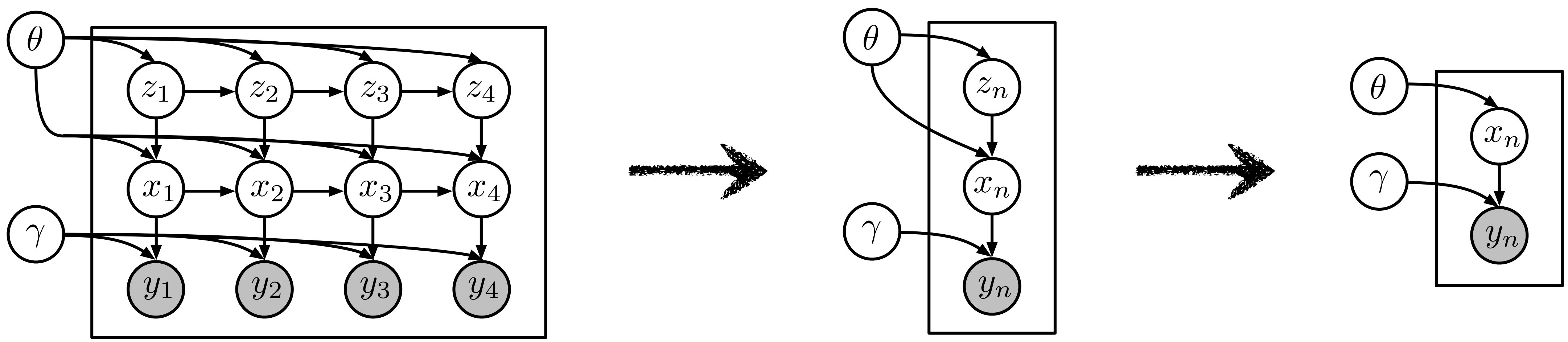

θ
γ
xn
yn

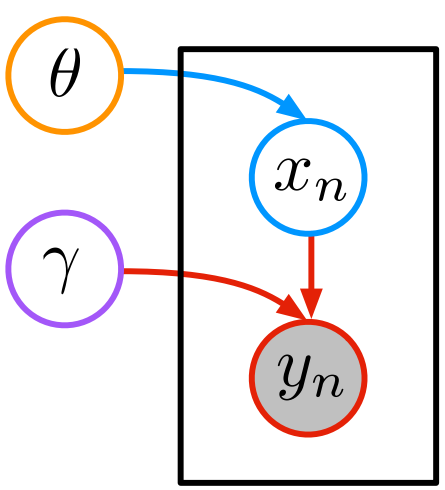




$p(\theta)$ conjugate prior on global variables

$p(x \mid \theta)$ exponential family on local variables

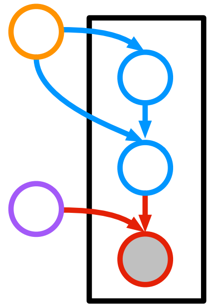




$p(\theta)$ conjugate prior on global variables

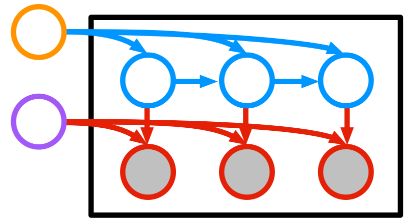
$p(x \mid \theta)$ exponential family on local variables

$p(y \mid x, \gamma)$ neural network observation model



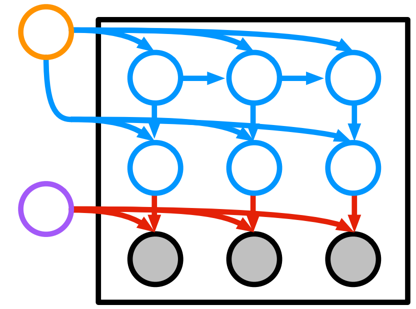
[1]

Gaussian mixture model



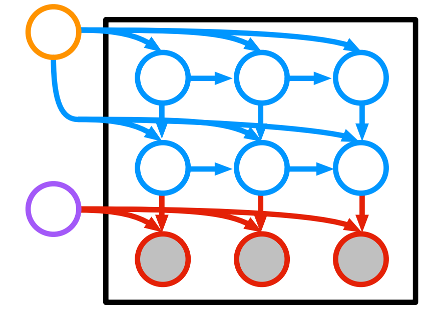
[2]

Linear dynamical system



[3]

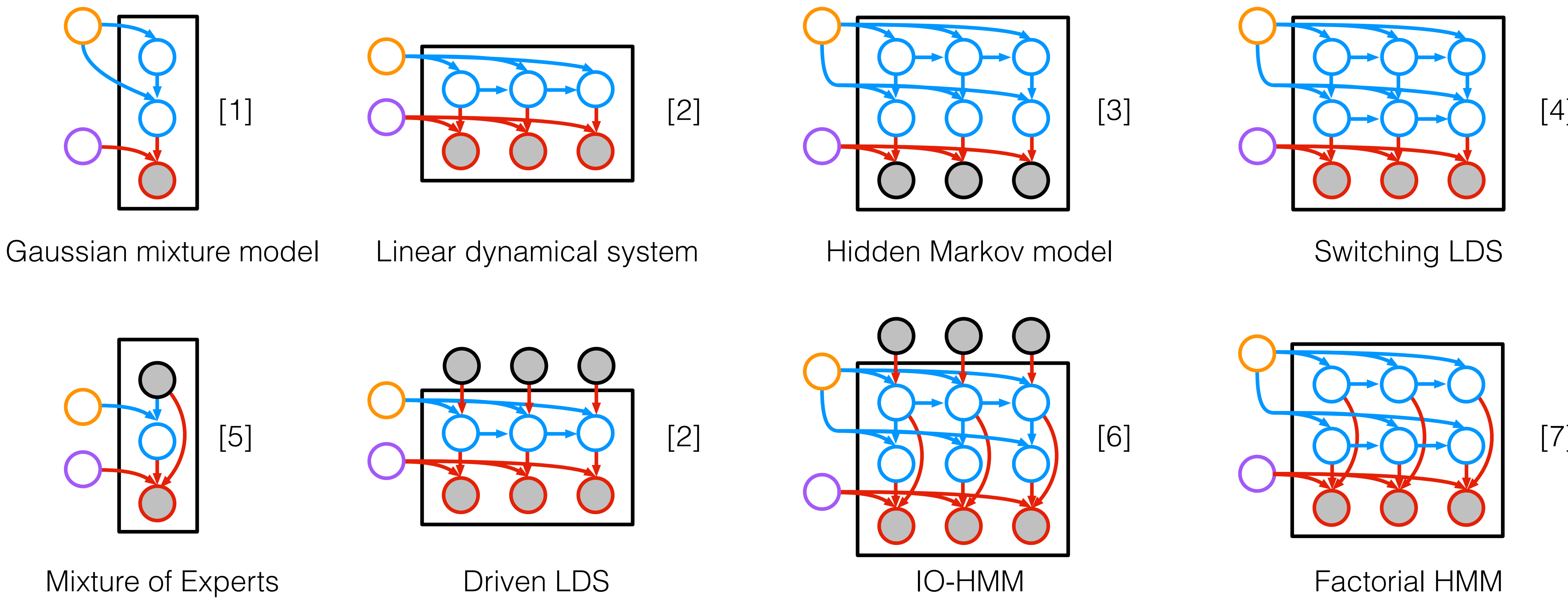
Hidden Markov model



[4]

Switching LDS

[1] Palmer, Wipf, Kreutz-Delgado, and Rao. Variational EM algorithms for non-Gaussian latent variable models. NIPS 2005.
[2] Ghahramani and Beal. Propagation algorithms for variational Bayesian learning. NIPS 2001.
[3] Beal. Variational algorithms for approximate Bayesian inference, Ch. 3. U of London Ph.D. Thesis 2003.
[4] Ghahramani and Hinton. Variational learning for switching state-space models. Neural Computation 2000.



[1] Palmer, Wipf, Kreutz-Delgado, and Rao. Variational EM algorithms for non-Gaussian latent variable models. NIPS 2005.
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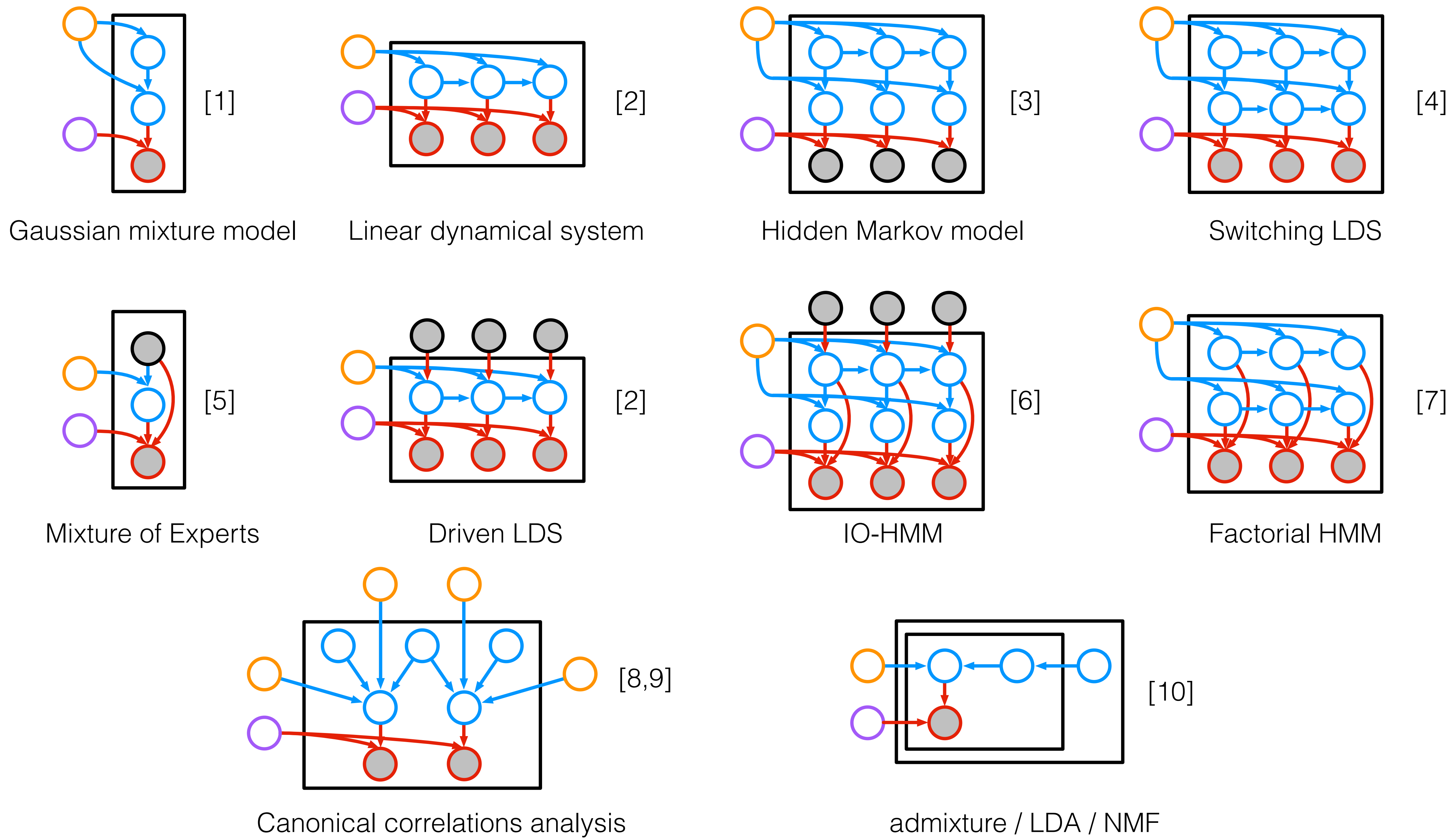
[4] Ghahramani and Hinton. Variational learning for switching state-space models. Neural Computation 2000.
[5] Jordan and Jacobs. Hierarchical Mixtures of Experts and the EM algorithm. Neural Computation 1994.
[6] Bengio and Frasconi. An Input Output HMM Architecture. NIPS 1995.
[7] Ghahramani and Jordan. Factorial Hidden Markov Models. Machine Learning 1997.



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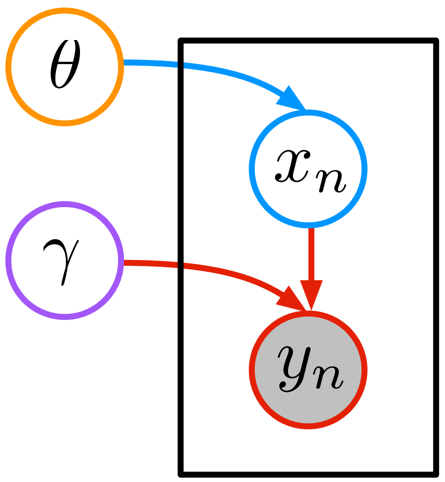
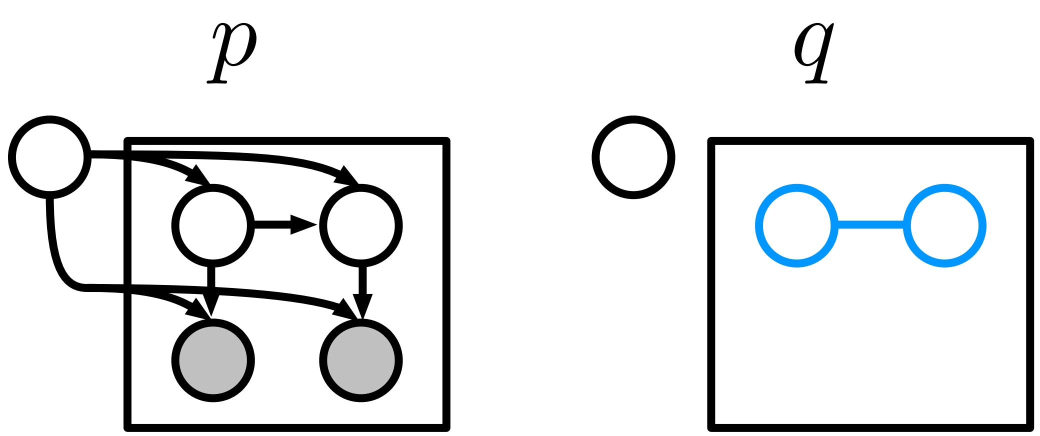
[4] Ghahramani and Hinton. Variational learning for switching state-space models. Neural Computation 2000.
[5] Jordan and Jacobs. Hierarchical Mixtures of Experts and the EM algorithm. Neural Computation 1994.
[6] Bengio and Frasconi. An Input Output HMM Architecture. NIPS 1995.
[7] Ghahramani and Jordan. Factorial Hidden Markov Models. Machine Learning 1997.
[8] Bach and Jordan. A probabilistic interpretation of Canonical Correlation Analysis. Tech. Report 2005.
[9] Archambeau and Bach. Sparse probabilistic projections. NIPS 2008.
[10] Hoffman, Bach, Blei. Online learning for Latent Dirichlet Allocation. NIPS 2010.



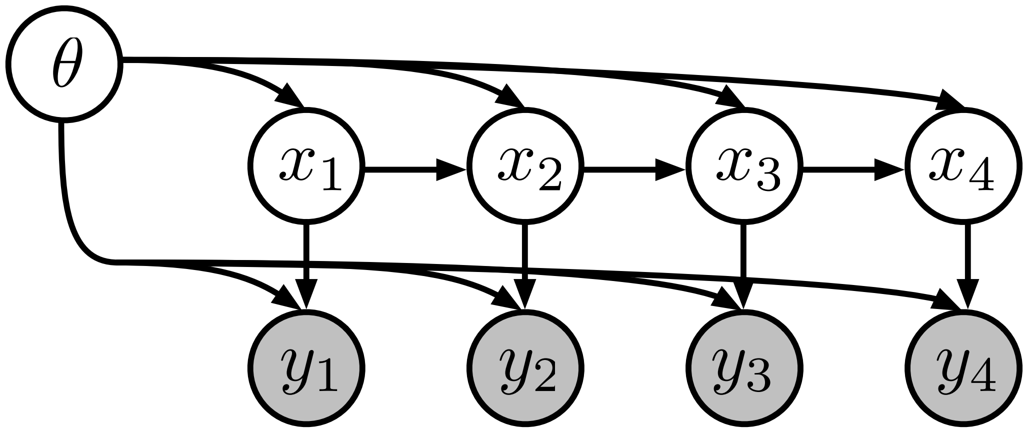
Inference?



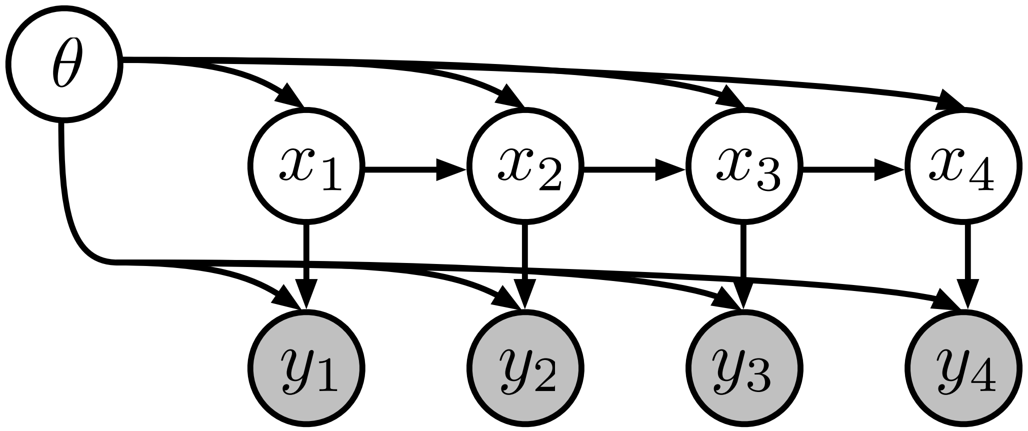
$$q^*(x) \triangleq \underset{q(x)}{\arg\max}\, \mathcal{L}[\, q(\theta)q(x)\,]$$

Natural gradient SVI
for nice exp. fam. PGMs [1,2]

[1] Hoffman, Bach, Blei. Online learning for Latent Dirichlet Allocation. NIPS 2010.
[2] Hoffman, Blei, Wang, and Paisley. Stochastic variational inference. JMLR 2013.



$p(x \mid \theta)$ is a linear dynamical system
$p(y \mid x, \theta)$ is a linear-Gaussian observation
$p(\theta)$ is a conjugate prior



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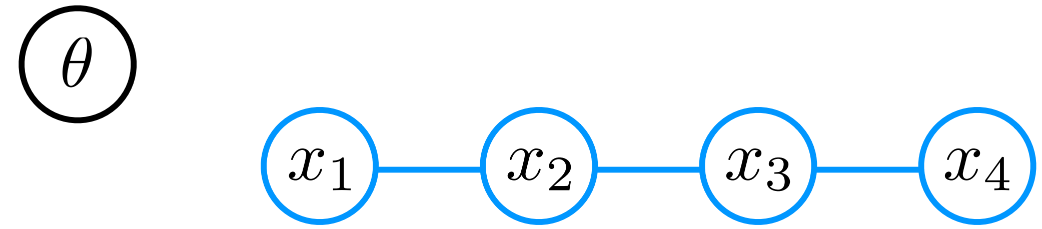
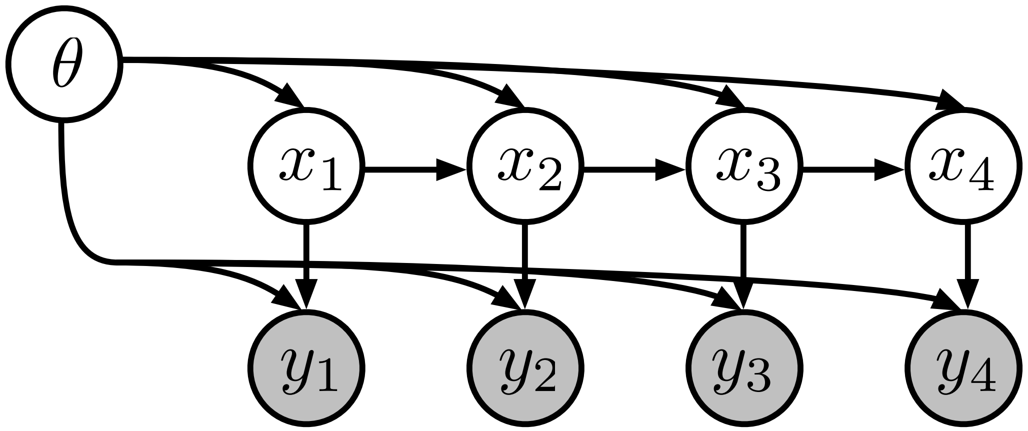
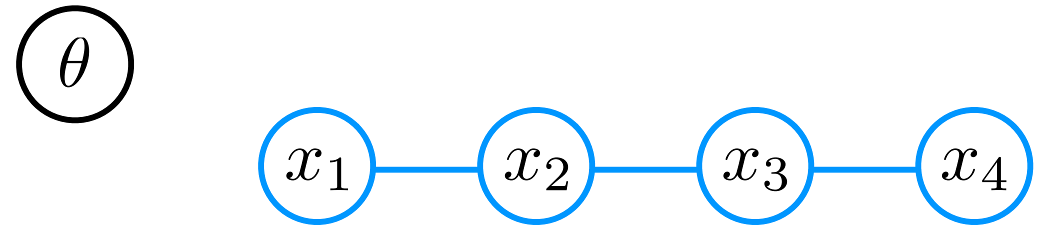


$$q(\theta)q(x) \approx p(\theta, x \mid y)$$





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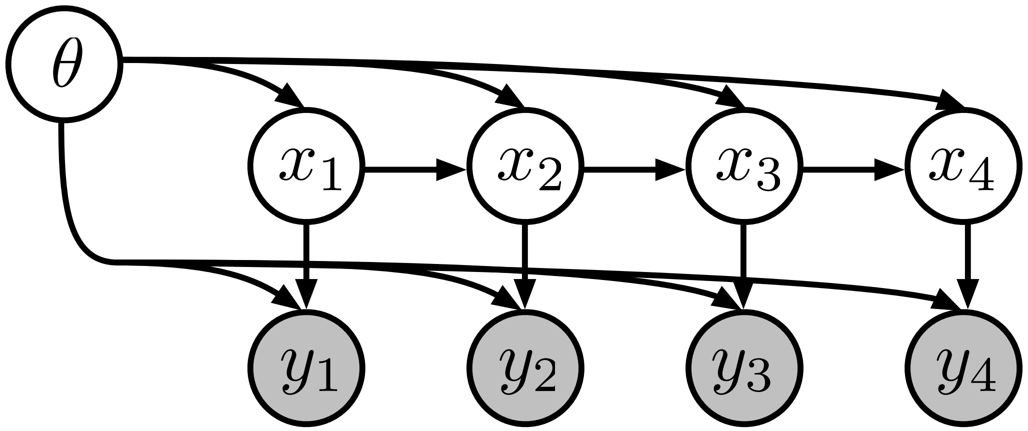

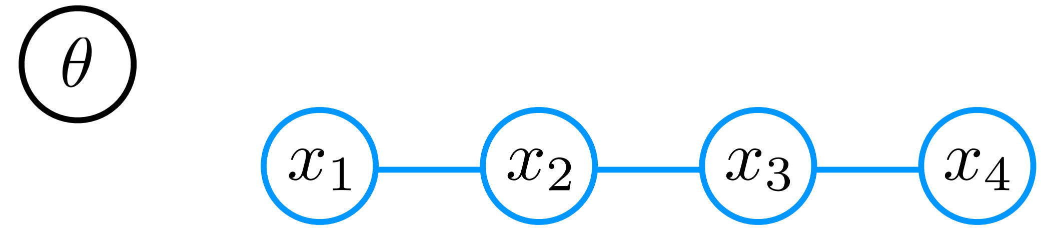

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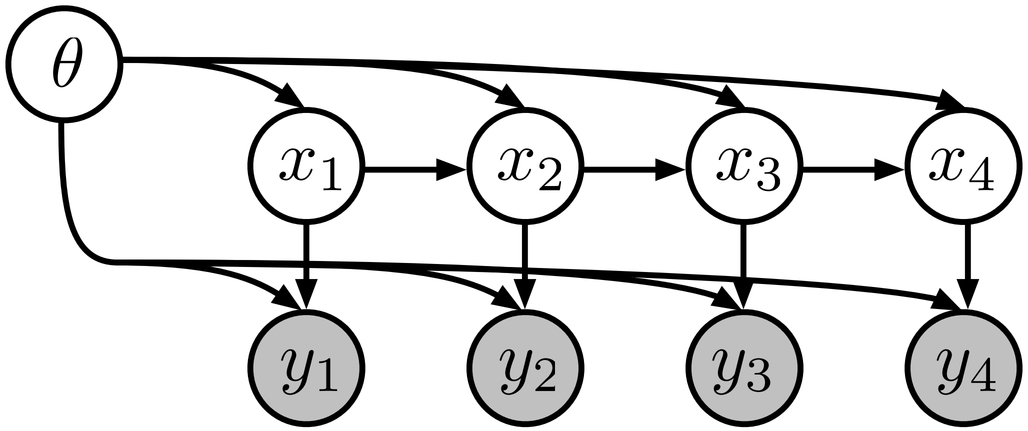

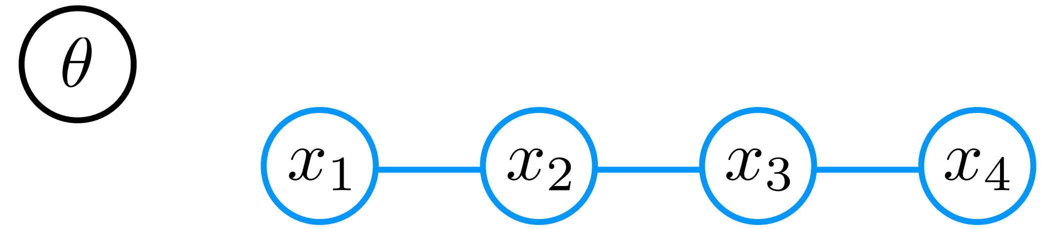

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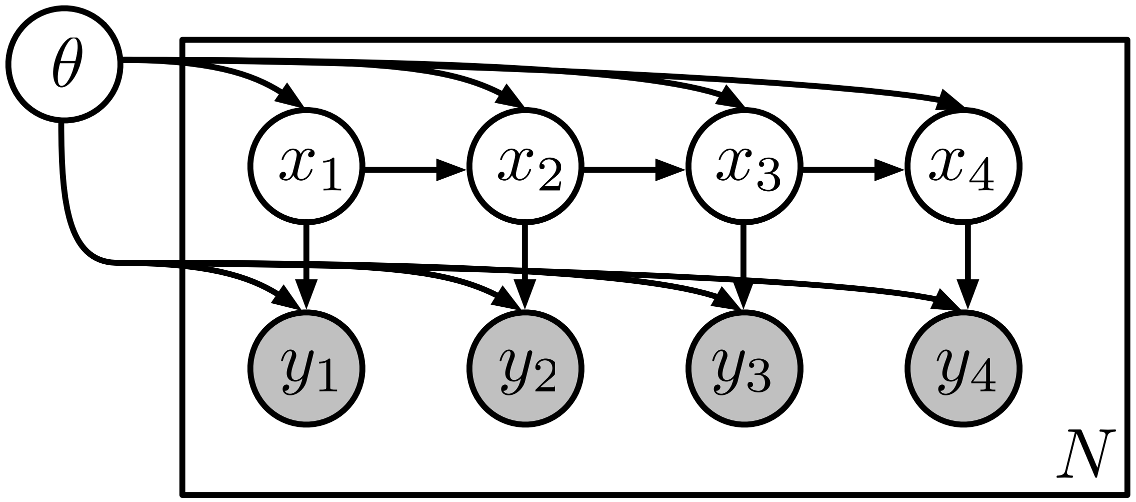
Proposition (natural gradient SVI of Hoffman et al. 2013)

$$\widetilde{\nabla}\mathcal{L}_{\text{SVI}}(\eta_\theta) = \eta_\theta^0 + \mathbb{E}_{q^*(x)}(t_{xy}(x,y), 1) - \eta_\theta$$



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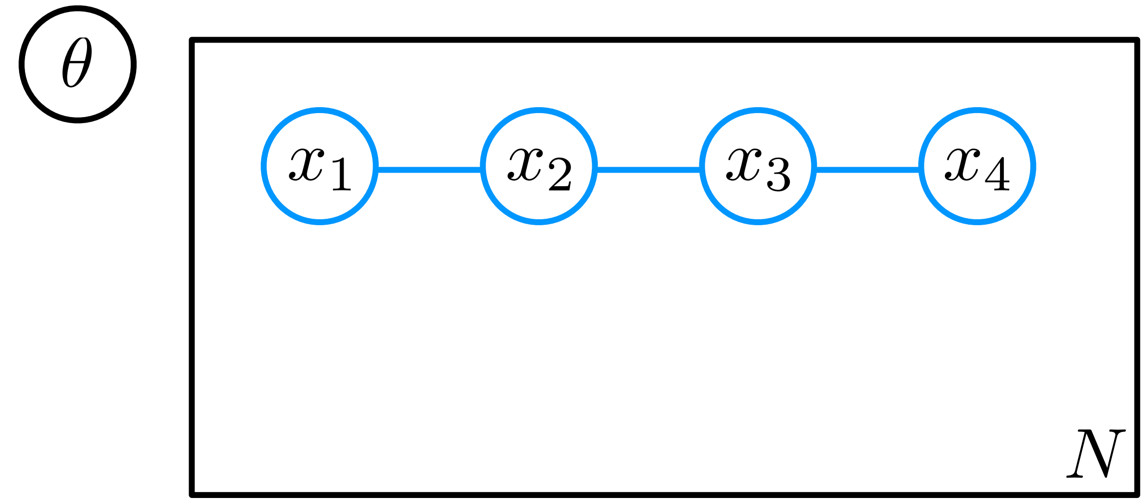

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Proposition (natural gradient SVI of Hoffman et al. 2013)

$$\widetilde{\nabla}\mathcal{L}_{\text{SVI}}(\eta_\theta) = \eta_\theta^0 + \sum_{n=1}^{N} \mathbb{E}_{q^*(x_n)}(t_{xy}(x_n, y_n), 1) - \eta_\theta$$

Step 1: compute evidence potentials

[1] **Johnson** and Willsky. Stochastic variational inference for Bayesian time series models. ICML 2014.
[2] Foti, Xu, Laird, and Fox. Stochastic variational inference for hidden Markov models. NIPS 2014.

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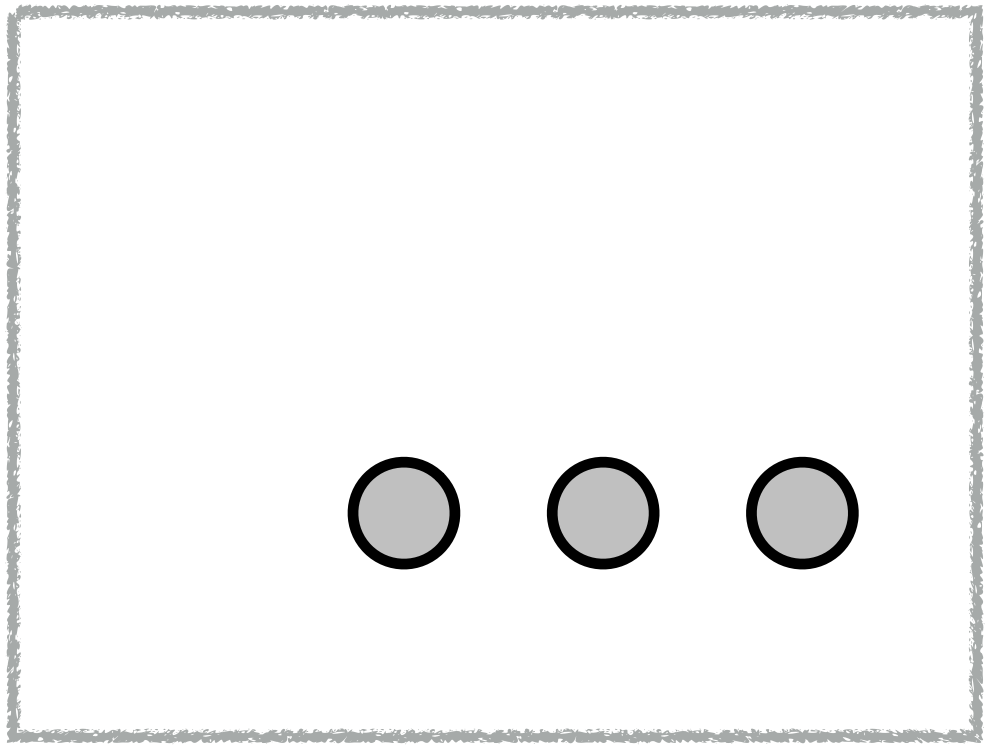

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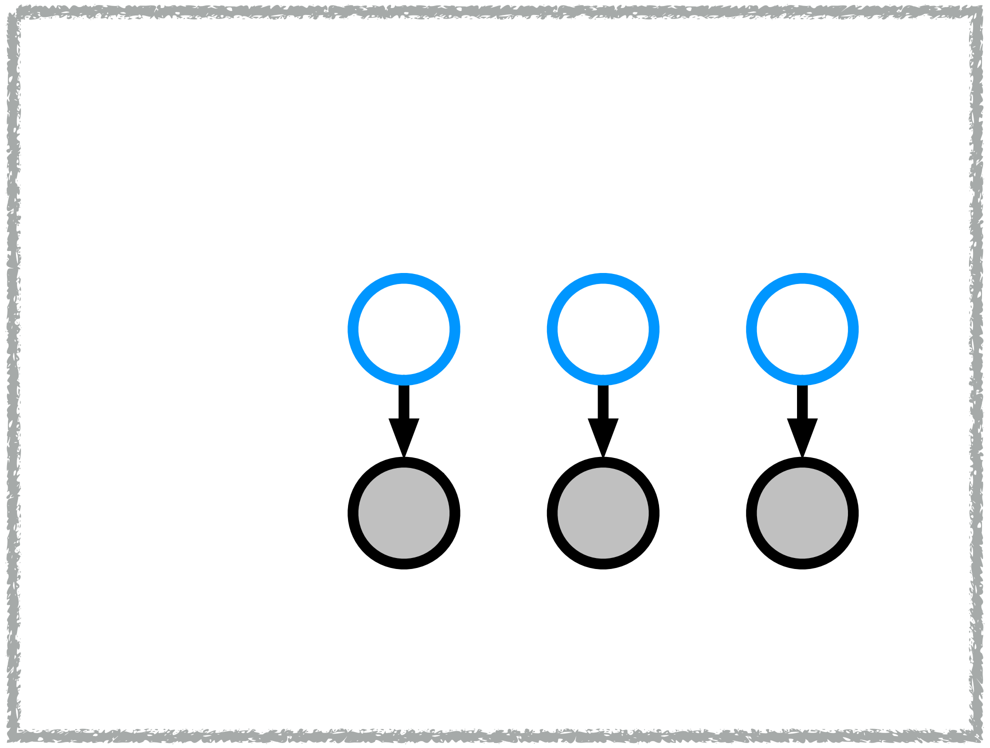

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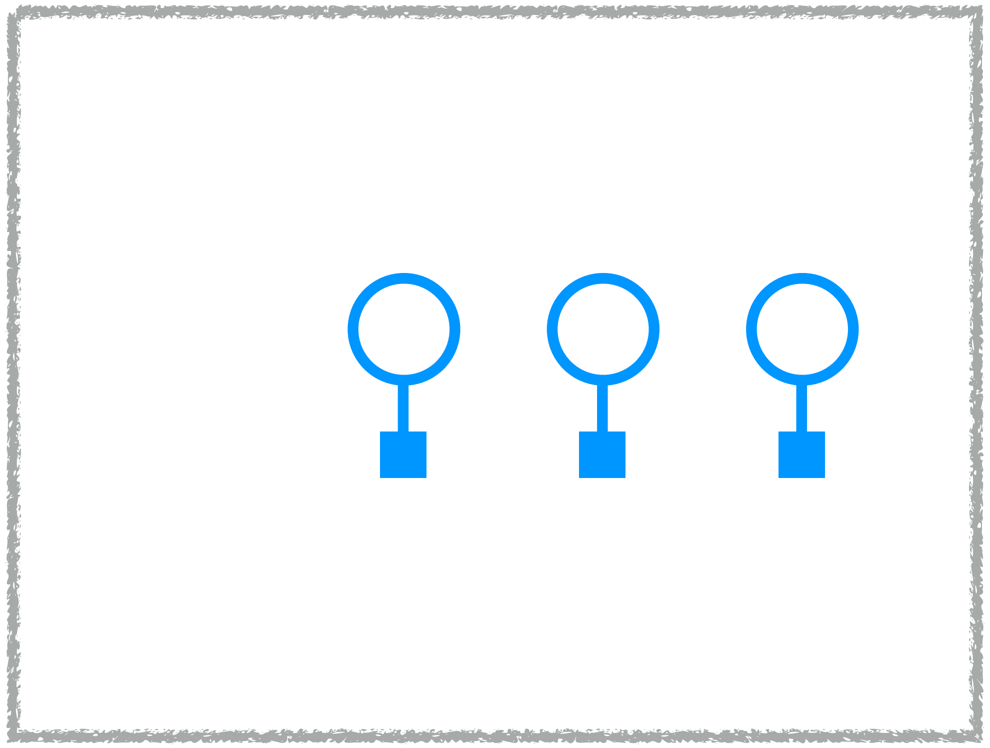

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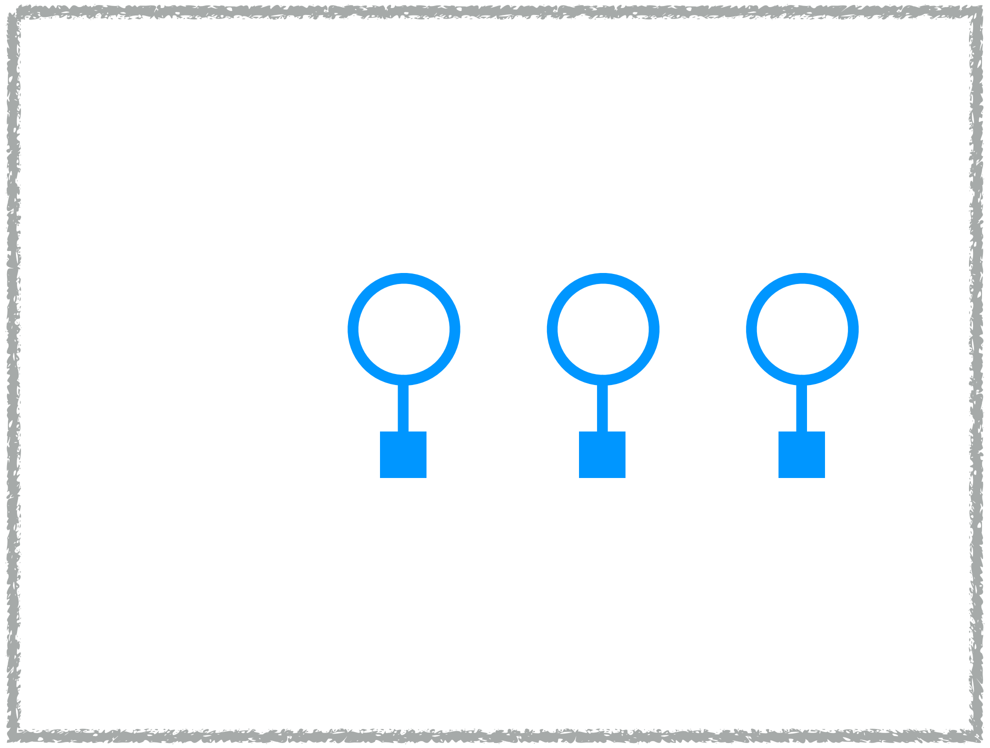

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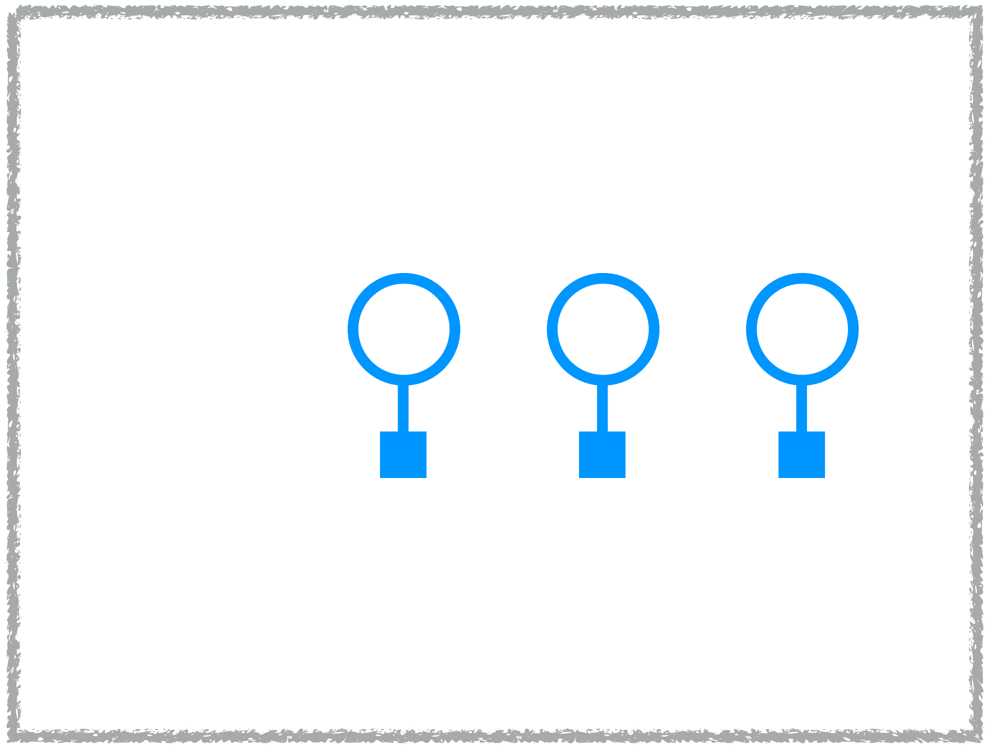

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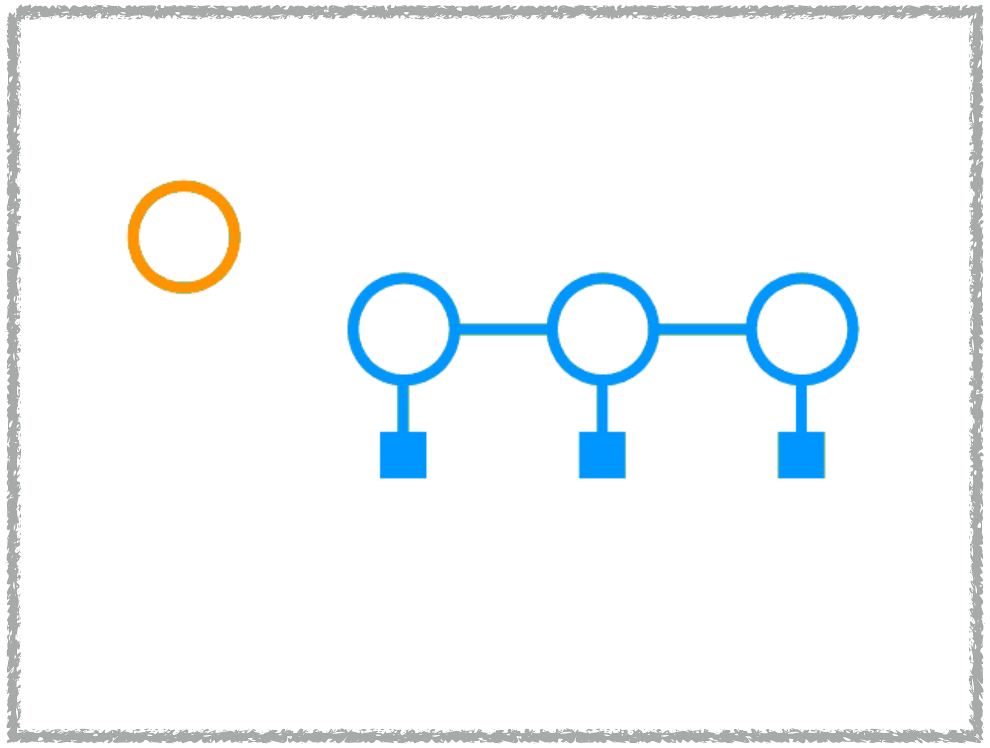

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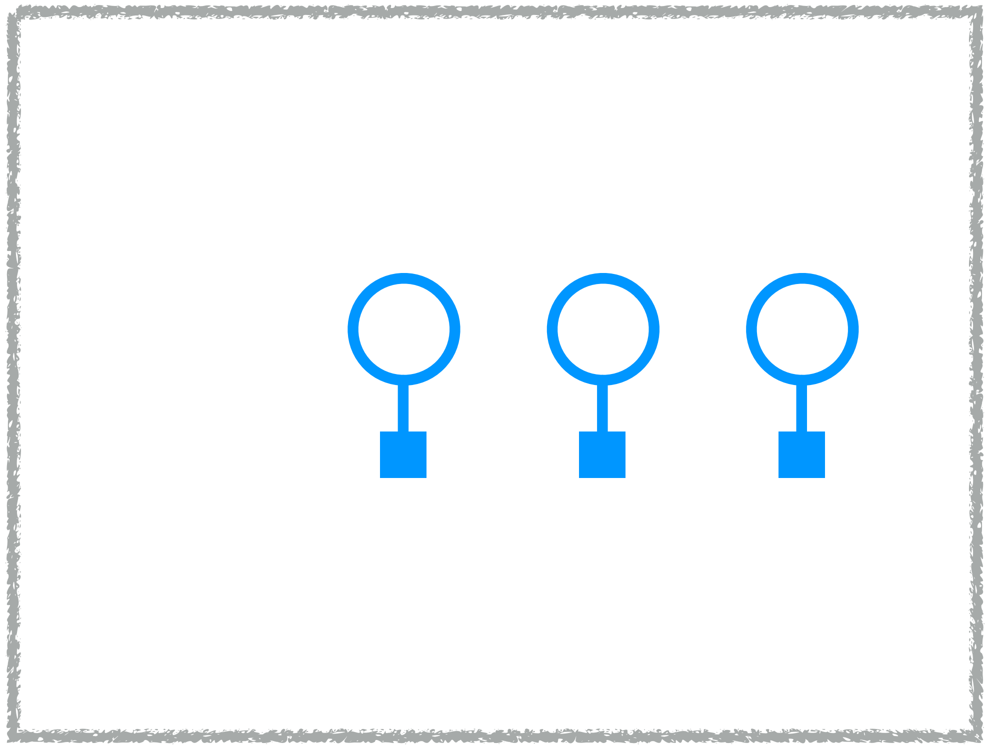

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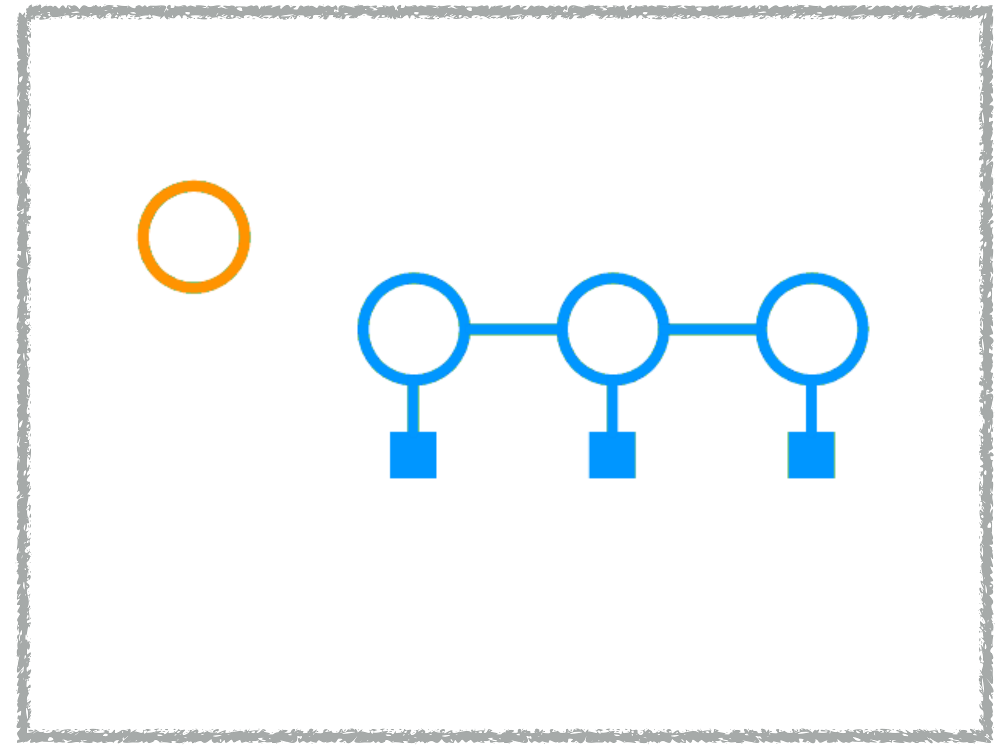
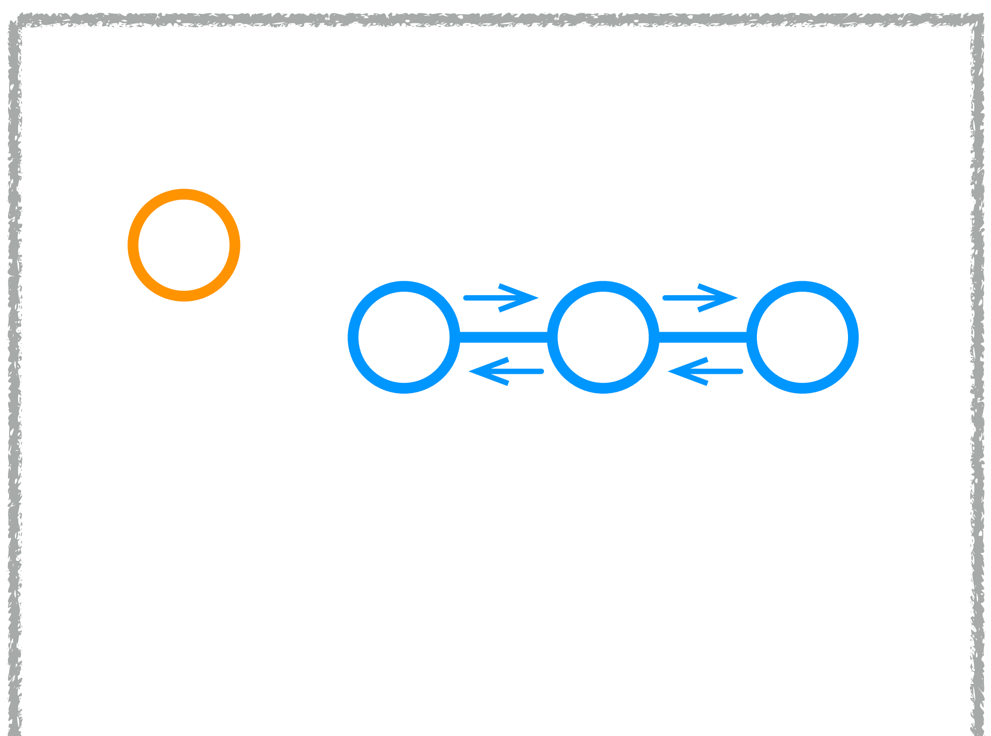


Step 3: compute natural gradient



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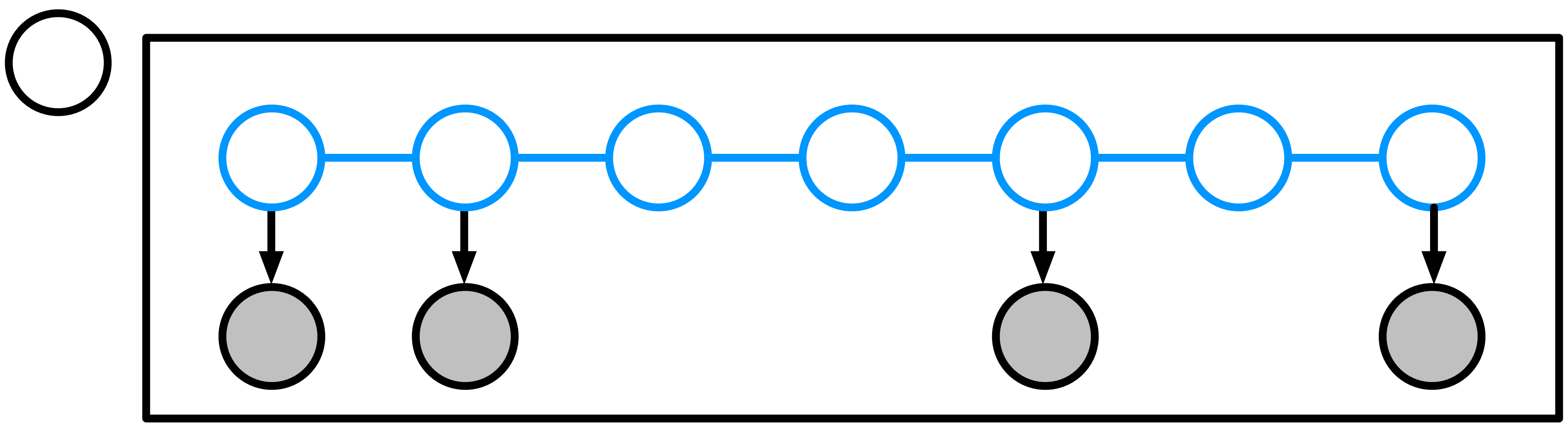
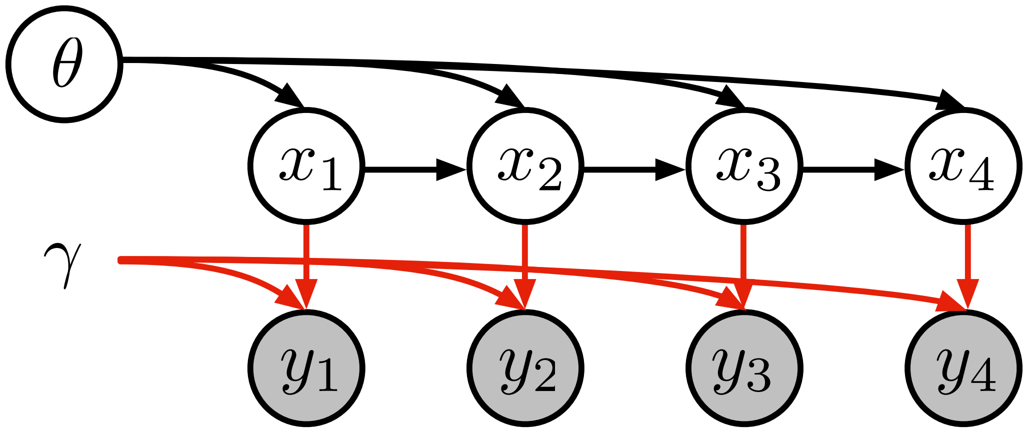
arbitrary inference queries

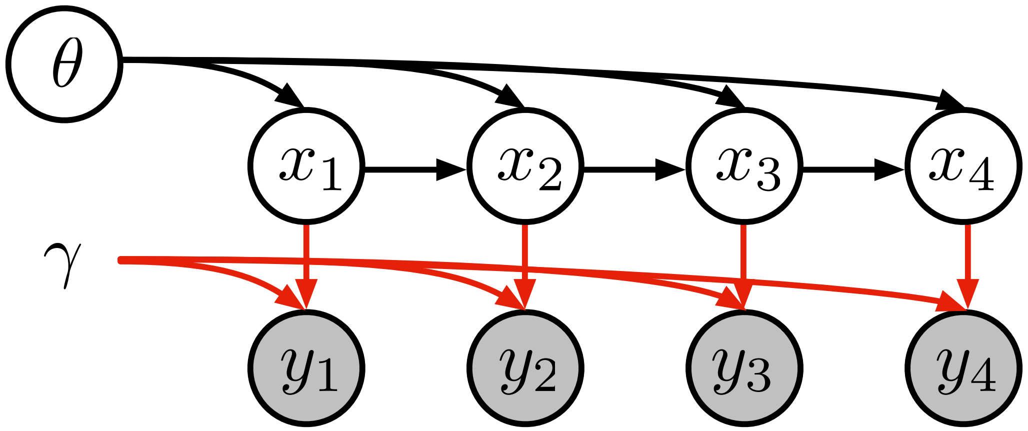


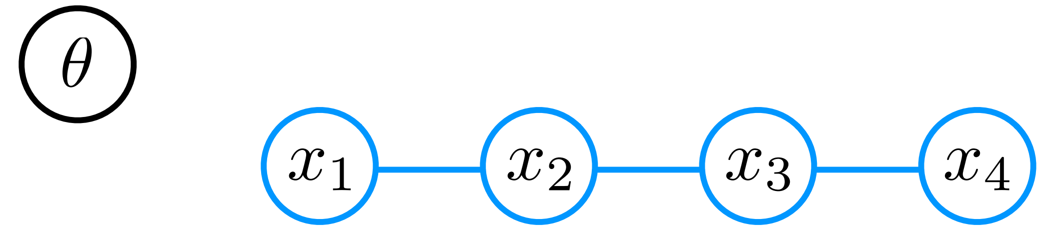


$p(x \mid \theta)$ is a linear dynamical system

$p(y \mid x, \gamma)$ is a neural network decoder

$p(\theta)$ is a conjugate prior





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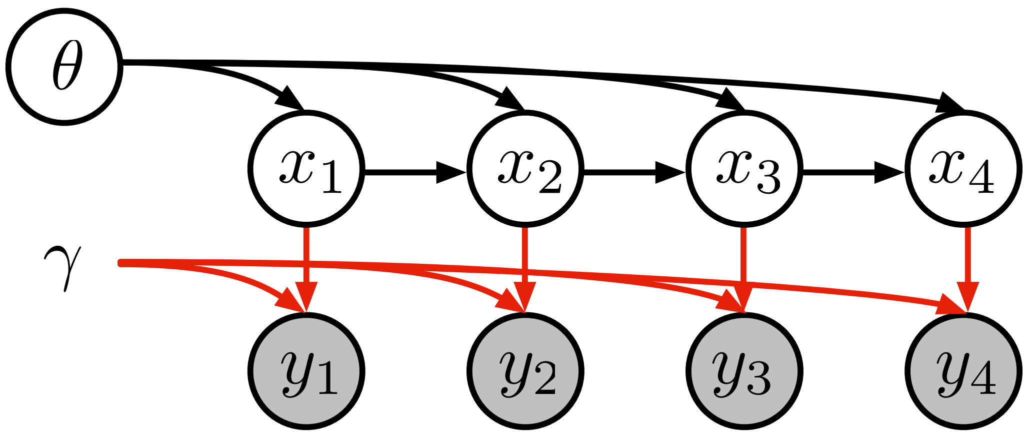

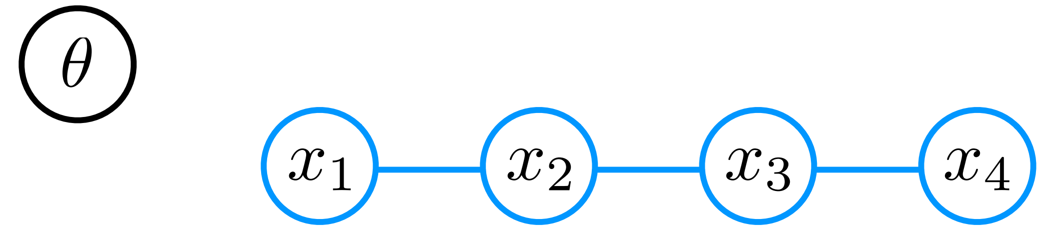

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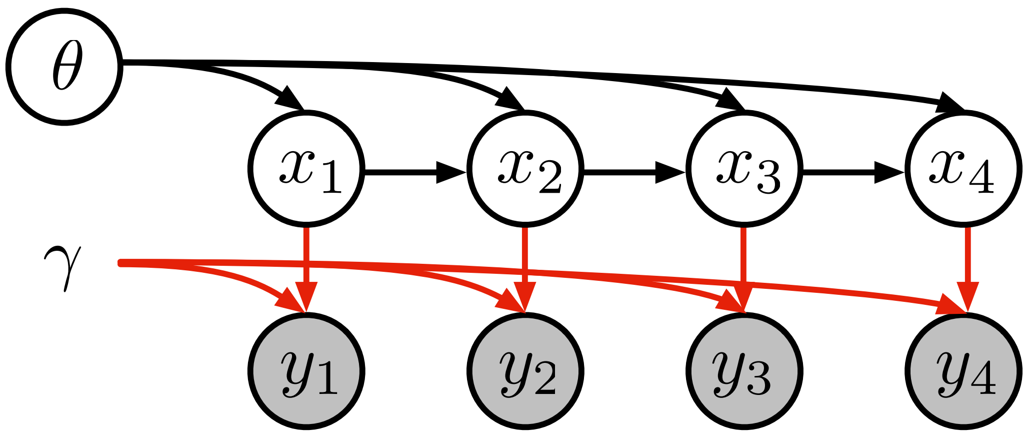

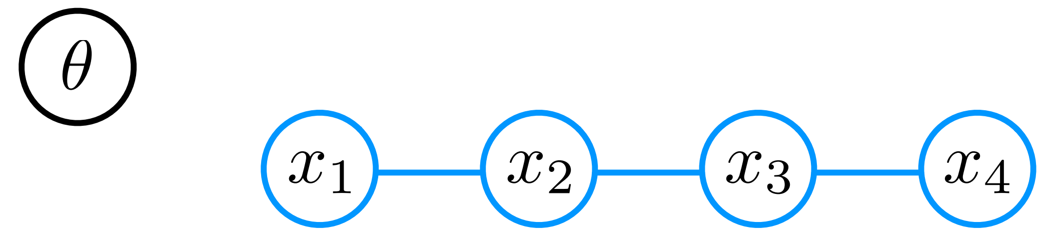

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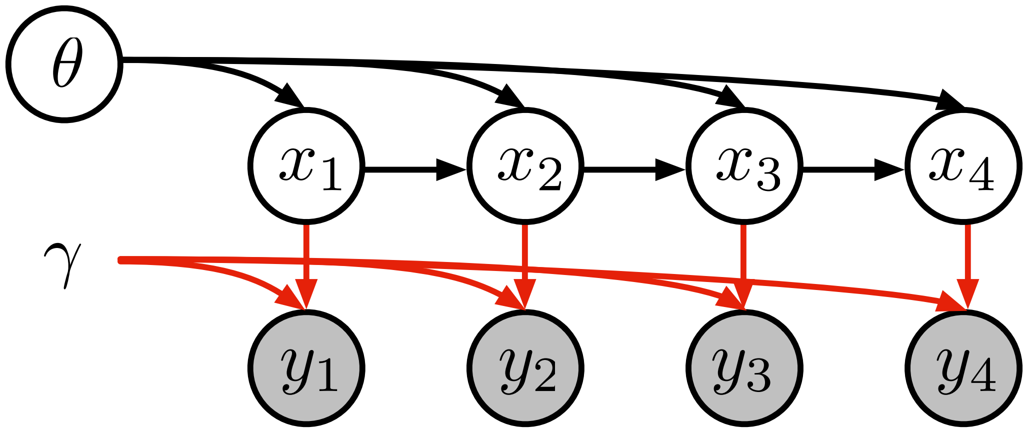

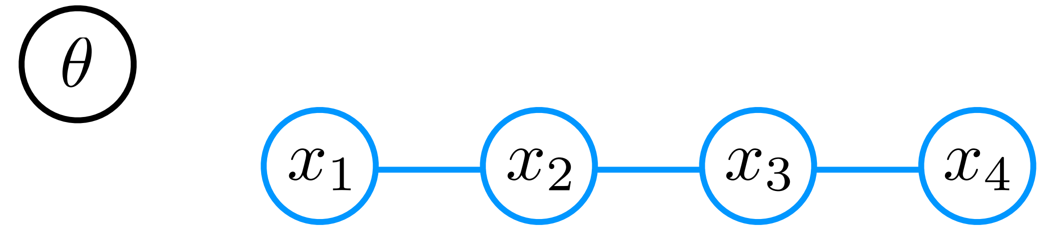

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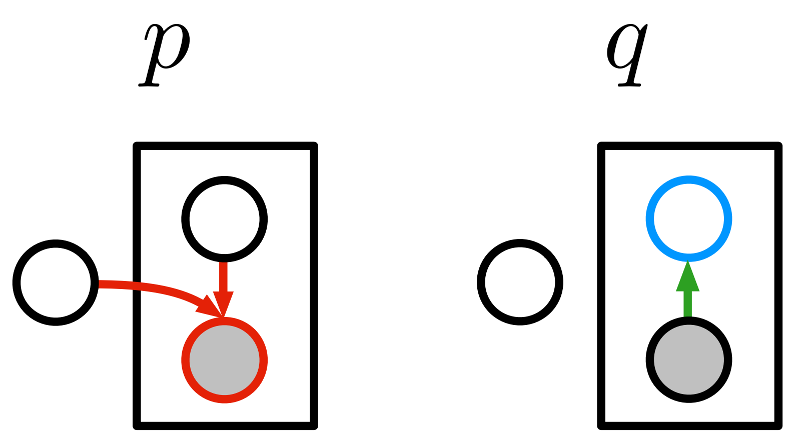
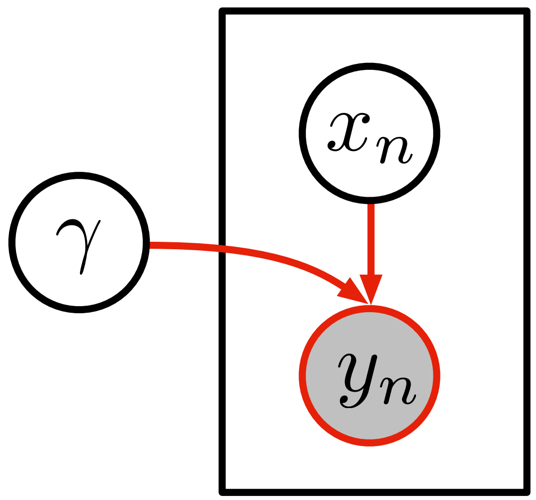


$$q^*(x) \triangleq \mathcal{N}(x \mid \mu(y;\phi), \Sigma(y;\phi))$$

Variational autoencoders and amortized inference [1,2]

[1] Kingma and Welling. Auto-encoding variational Bayes. ICLR 2014.
[2] Rezende, Mohamed, and Wierstra. Stochastic backpropagation and approximate inference in deep generative models. ICML 2014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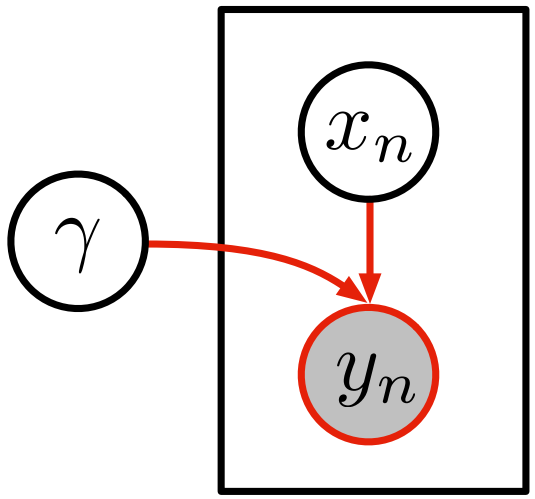
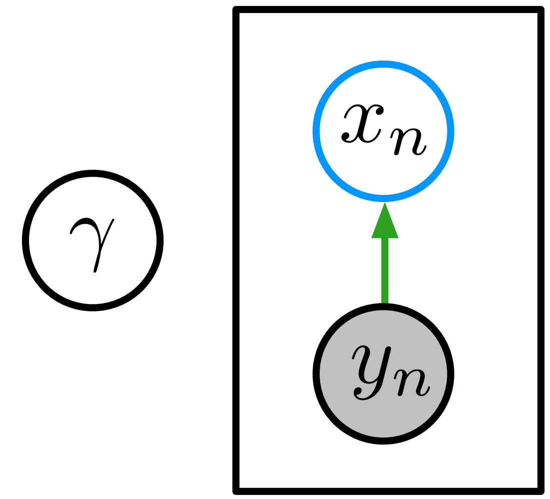
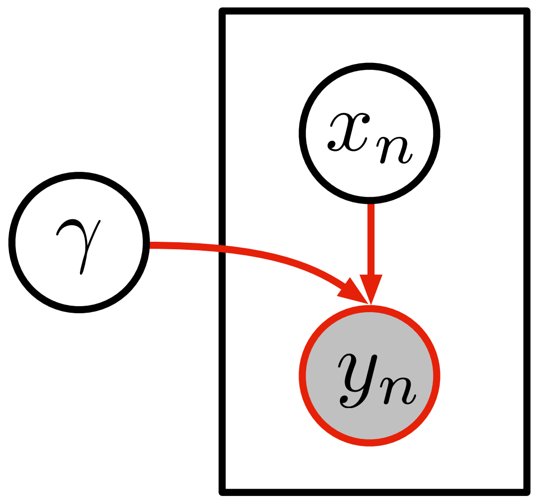
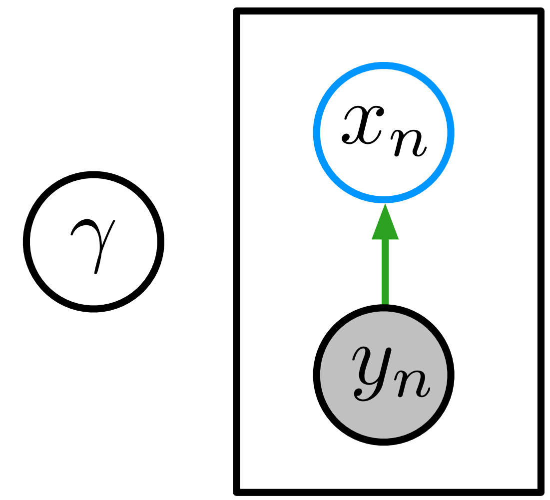




$$q^{\star}(x_n) \triangleq \mathcal{N}(x_n \mid \mu(y_n;\phi),\ \Sigma(y_n;\phi))$$





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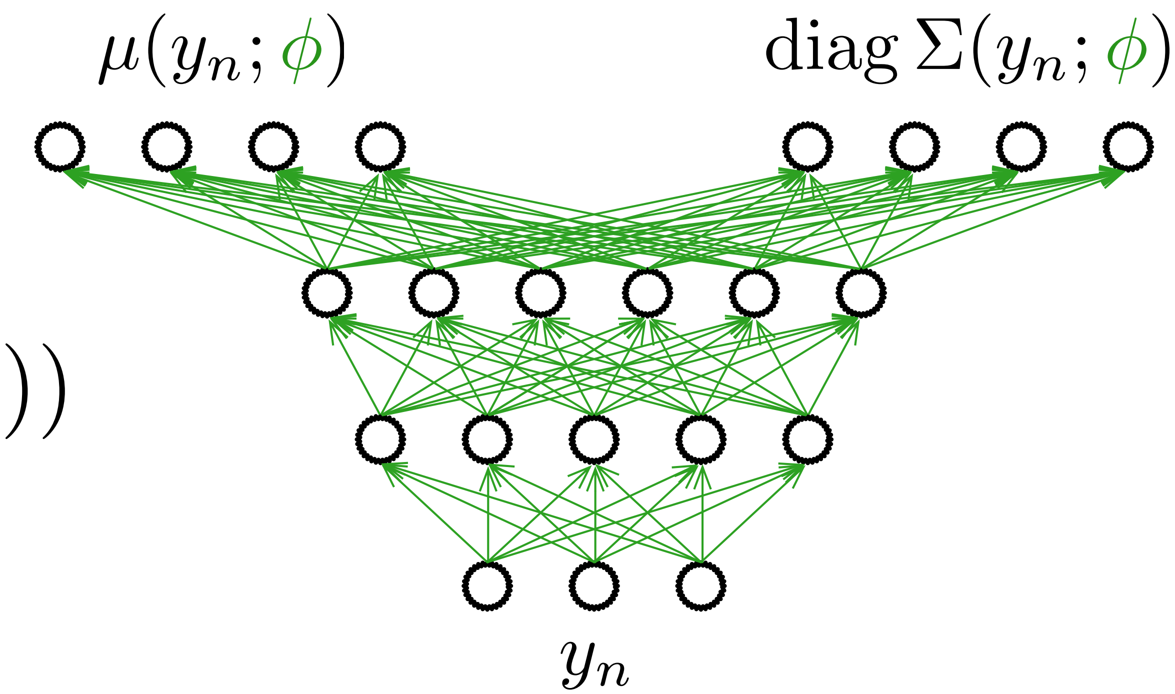

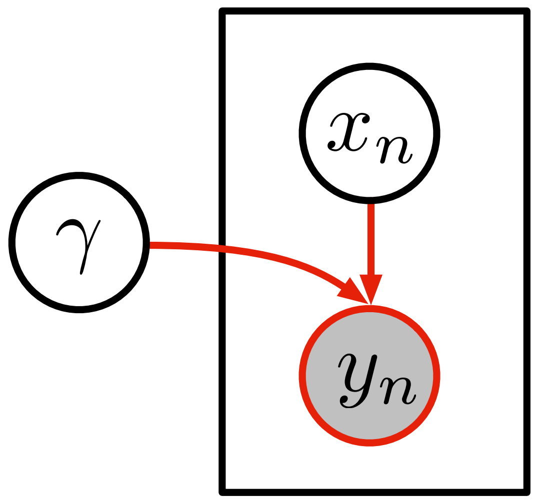

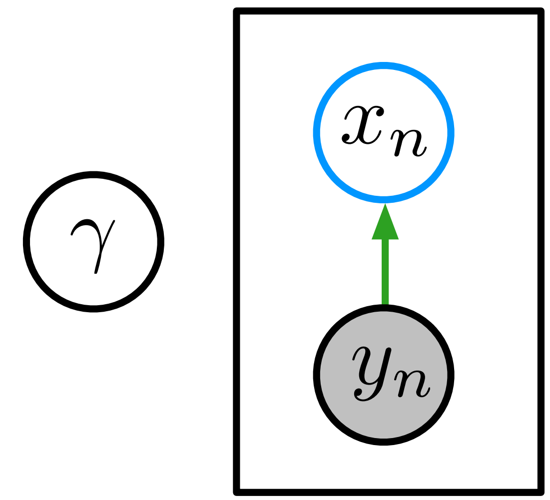

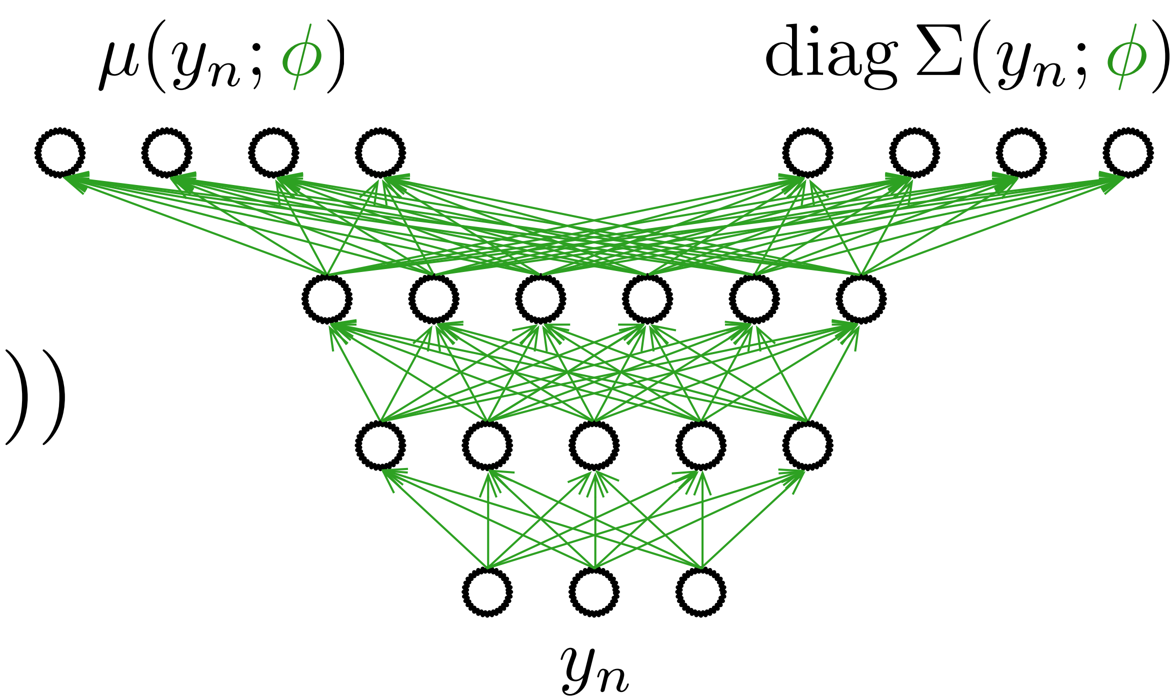

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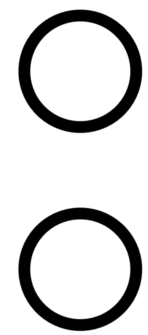
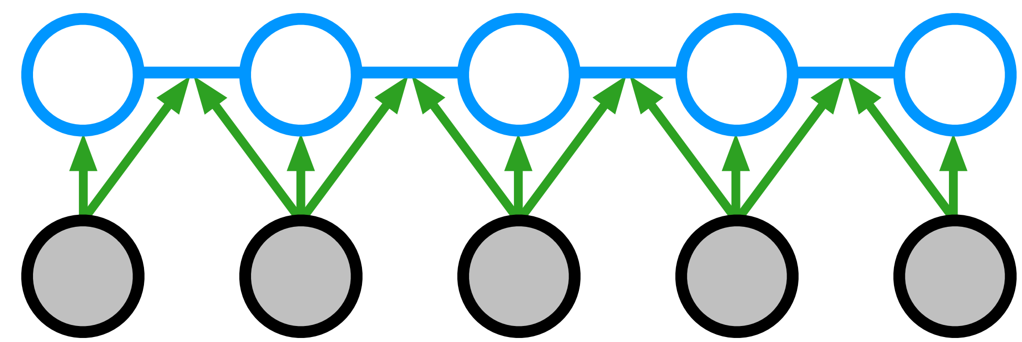
$$\mathcal{L}_{\mathrm{VAE}}(\eta_\gamma, \phi) \triangleq \mathcal{L}(\eta_\gamma, \eta_x^\star(\phi))$$

$$\mu_t(y_t; \phi_\mu)$$

[1,2] $$J_{t,t}(y_t; \phi_D)$$

$$J_{t,t+1}(y_t, y_{t+1}; \phi_B)$$





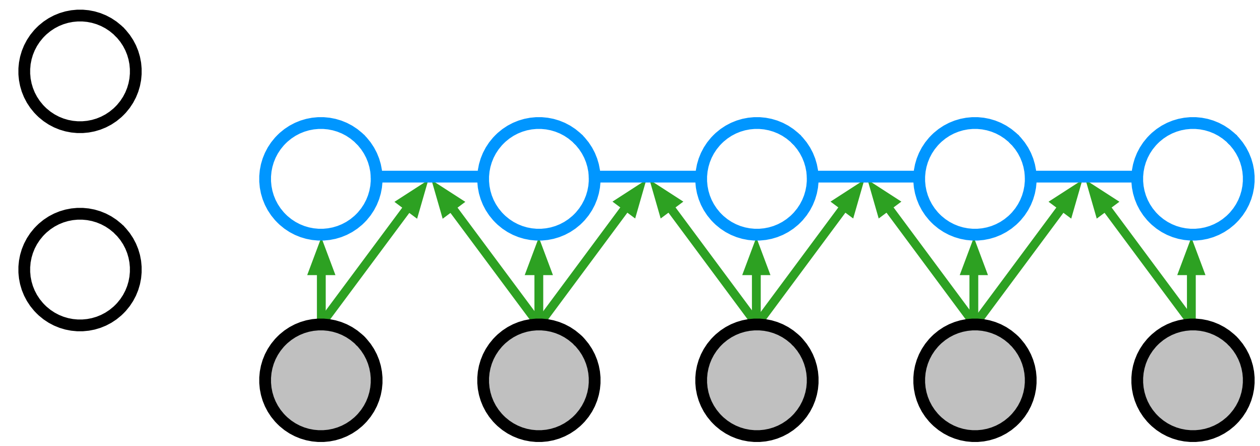
[1] Archer, Park, Buesing, Cunningham, Paninski. Black box variational inference for state space models. ICLR 2016 Workshops.
[2] Gao*, Archer*, Paninski, Cunningham. Linear dynamical neural population models through nonlinear embeddings. NIPS 2016.

[1,2]

$$\mu_t(y_t;\phi_\mu)$$

$$J_{t,t}(y_t;\phi_D)$$

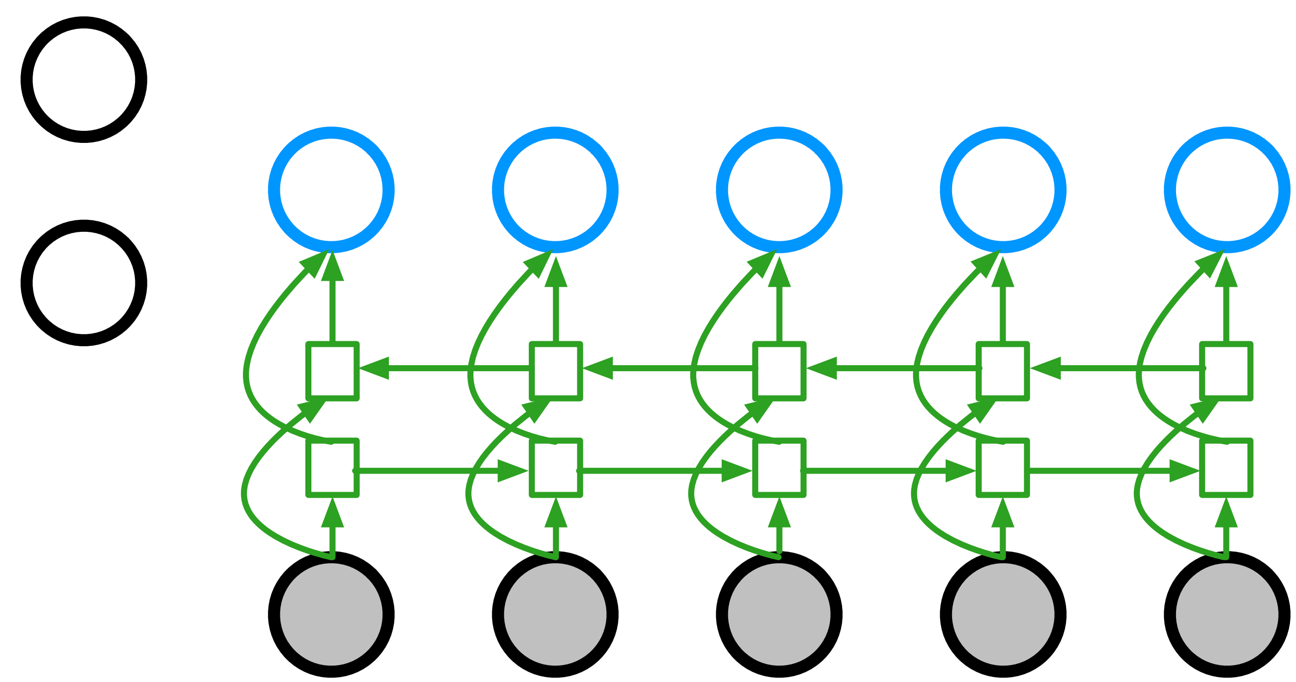
$$J_{t,t+1}(y_t,y_{t+1};\phi_B)$$



[3]

$$\mu_t(y_{1:T},\hat{x}_{t-1};\phi)$$

$$\Sigma_t(y_{1:T},\hat{x}_{t-1};\phi)$$



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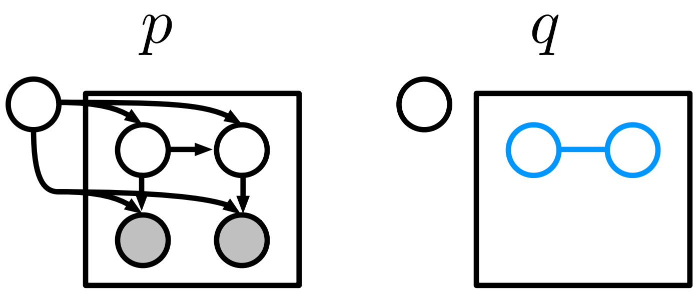
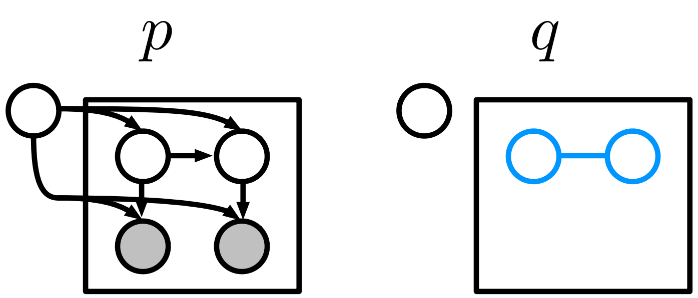
[3] Krishnan, Shalit, Sontag. Structured inference networks for nonlinear state space models. AISTATS 2017.



$$q^*(x) \triangleq \arg\max_{q(x)} \mathcal{L}[\, q(\theta)q(x) \,]$$

Natural gradient SVI



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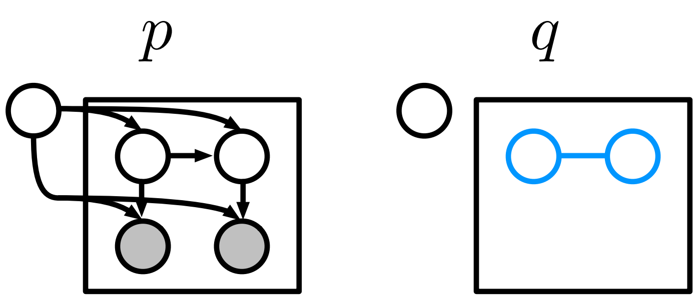
Natural gradient SVI

– expensive for general obs.

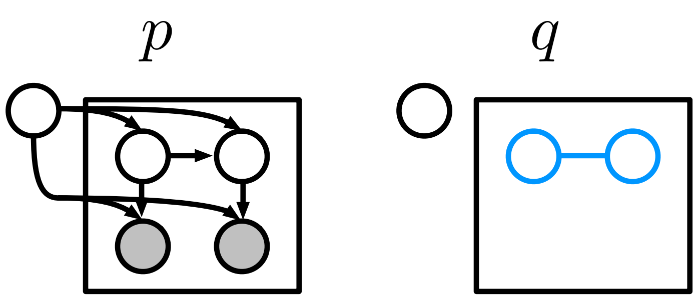


$$q^*(x) \triangleq \arg\max_{q(x)} \mathcal{L}[\, q(\theta) q(x) \,]$$

Natural gradient SVI

− expensive for general obs.

+ optimal local factor



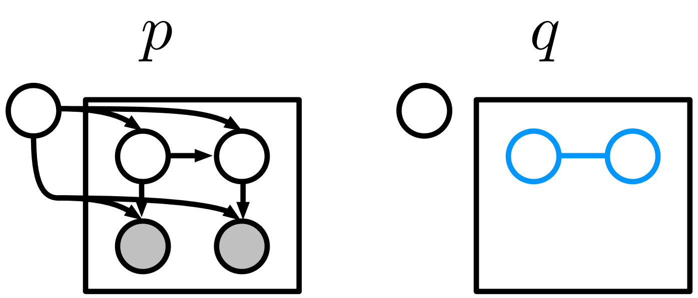
$$q^*(x) \triangleq \arg\max_{q(x)} \mathcal{L}[\, q(\theta)q(x)\,]$$

Natural gradient SVI

– expensive for general obs.

\+ optimal local factor

\+ exploits conj. graph structure



$$q^*(x) \triangleq \arg\max_{q(x)} \mathcal{L}[\, q(\theta) q(x) \,]$$

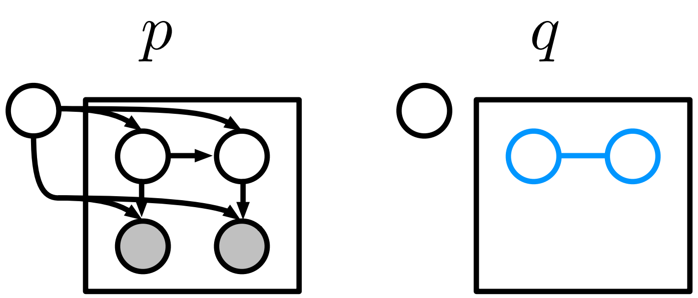
Natural gradient SVI

– expensive for general obs.

+ optimal local factor

+ exploits conj. graph structure

+ arbitrary inference queries



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Natural gradient SVI

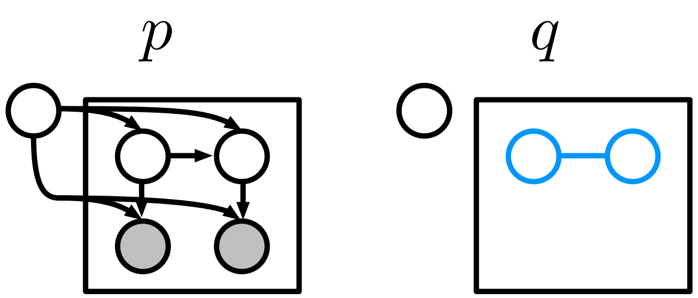
– expensive for general obs.

+ optimal local factor

+ exploits conj. graph structure

+ arbitrary inference queries

+ natural gradients



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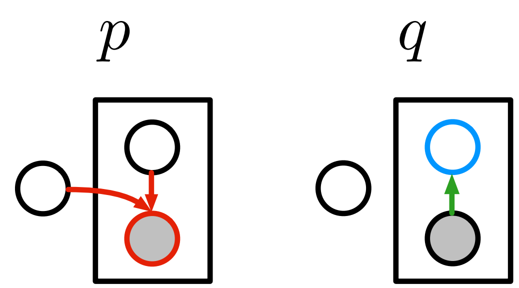
Natural gradient SVI



$$q^*(x) \triangleq \mathcal{N}(x \mid \mu(y;\phi), \Sigma(y;\phi))$$

Variational autoencoders

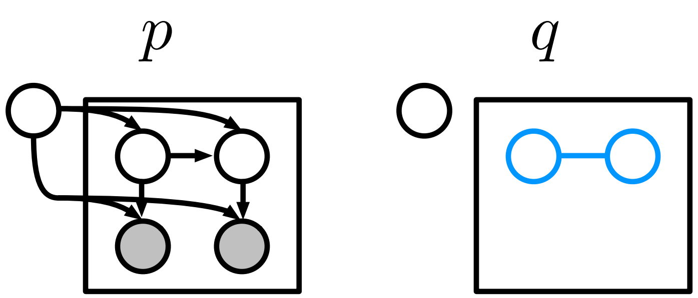
– expensive for general obs.

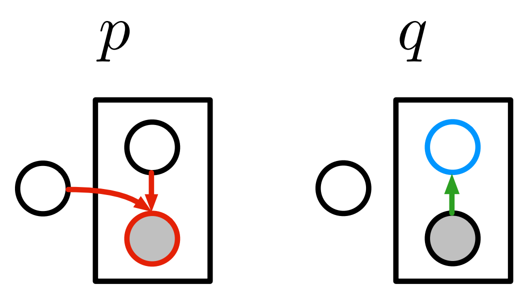
\+ optimal local factor

\+ exploits conj. graph structure

\+ arbitrary inference queries

\+ natural gradients





$$q^*(x) \triangleq \arg\max_{q(x)} \mathcal{L}[\, q(\theta) q(x) \,]$$

$$q^*(x) \triangleq \mathcal{N}(x \,|\, \mu(y;\phi), \Sigma(y;\phi))$$

Natural gradient SVI

– expensive for general obs.

+ optimal local factor

+ exploits conj. graph structure

+ arbitrary inference queries

+ natural gradients

Variational autoencoders

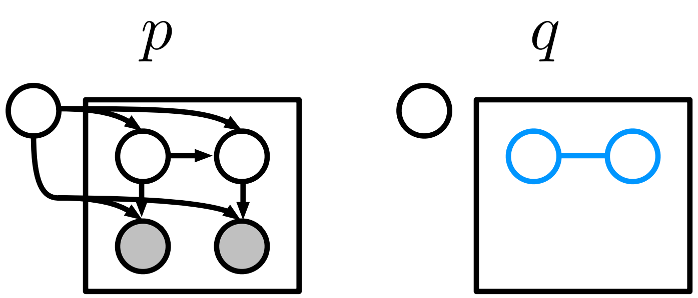
+ fast for general obs.

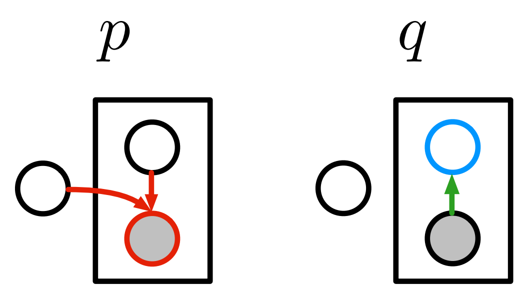
– suboptimal local inference

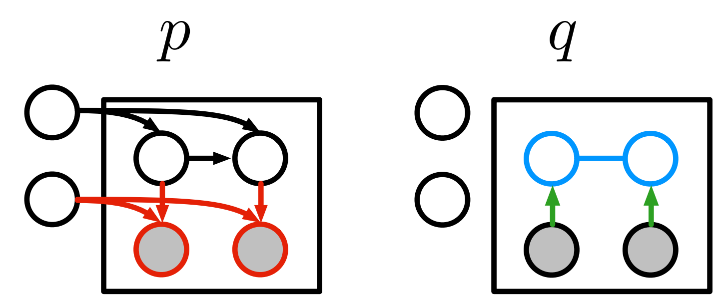
– ϕ does all local inference

– limited inference queries

– no cheap natural gradients







$$q^*(x) \triangleq \underset{q(x)}{\arg\max}\, \mathcal{L}[\, q(\theta)q(x)\,]$$

$$q^*(x) \triangleq \mathcal{N}(x \mid \mu(y;\phi), \Sigma(y;\phi))$$

$$q^*(x) \triangleq \ ?$$

Natural gradient SVI

- – expensive for general obs.
- + optimal local factor
- + exploits conj. graph structure
- + arbitrary inference queries
- + natural gradients

Variational autoencoders

- + fast for general obs.
- – suboptimal local inference
- – ϕ does all local inference
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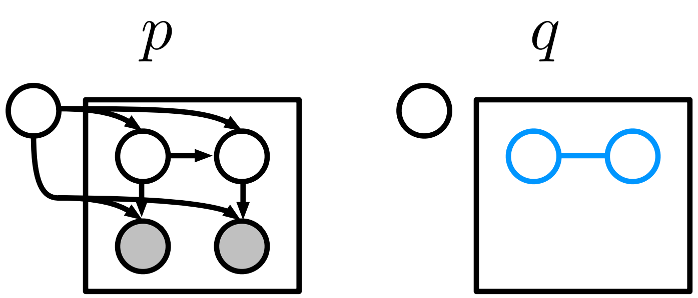
- – no cheap natural gradients

Structured VAEs [1]

[1] **Johnson**, Duvenaud, Wiltschko, Datta, and Adams. Composing graphical models and neural networks. NIPS 2016.



$$q^*(x) \triangleq \arg\max_{q(x)} \mathcal{L}[\, q(\theta)q(x)\,]$$

Natural gradient SVI

- – expensive for general obs.
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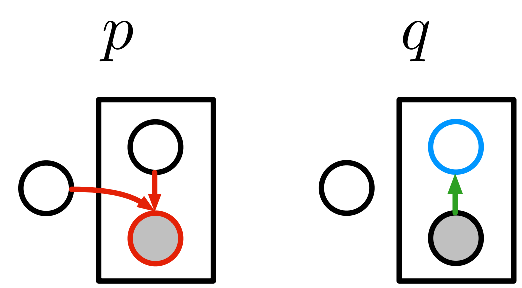

$$q^*(x) \triangleq \mathcal{N}(x \,|\, \mu(y;\phi), \Sigma(y;\phi))$$

Variational autoencoders

- + fast for general obs.
- – suboptimal local inference
- – ϕ does all local inference
- – limited inference queries
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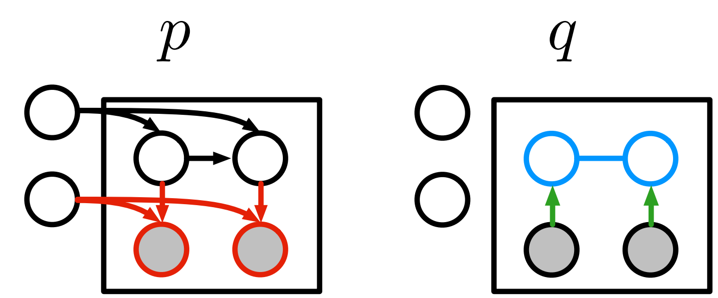


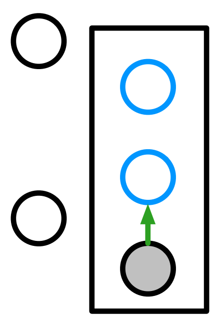
$$q^*(x) \triangleq \; ?$$

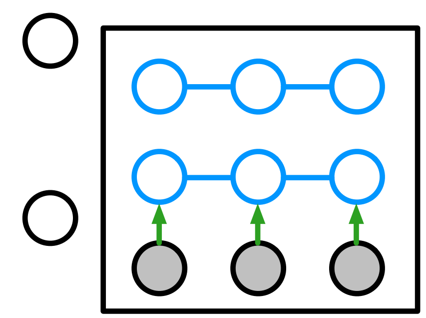
Structured VAEs [1]

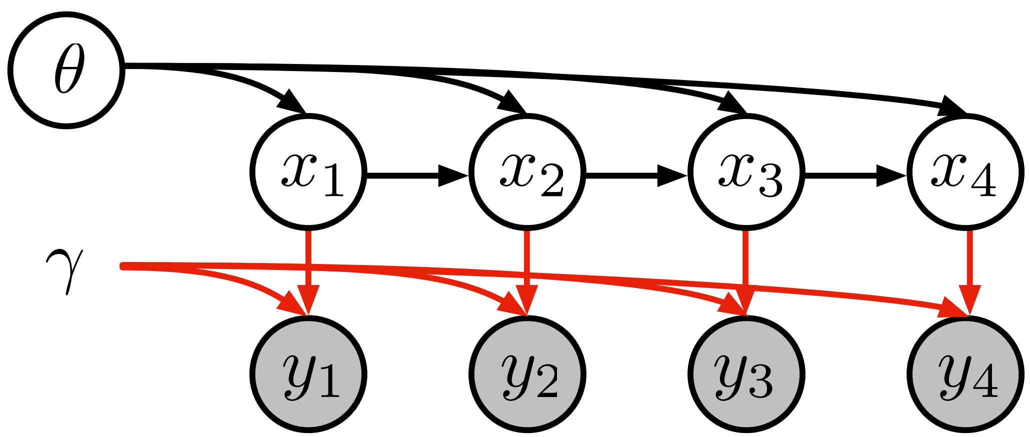
- + fast for general obs.
- ± optimal given conj. evidence
- + exploits conj. graph structure
- + arbitrary inference queries
- + natural gradients on η_θ

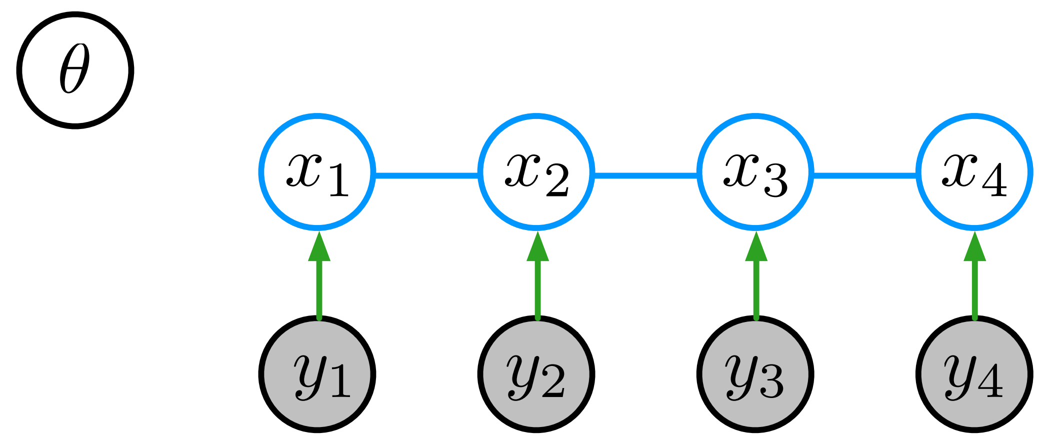
[1] **Johnson**, Duvenaud, Wiltschko, Datta, and Adams. Composing graphical models and neural networks. NIPS 2016.

Inference: recognition networks output conjugate potentials, then apply fast graphical model inference

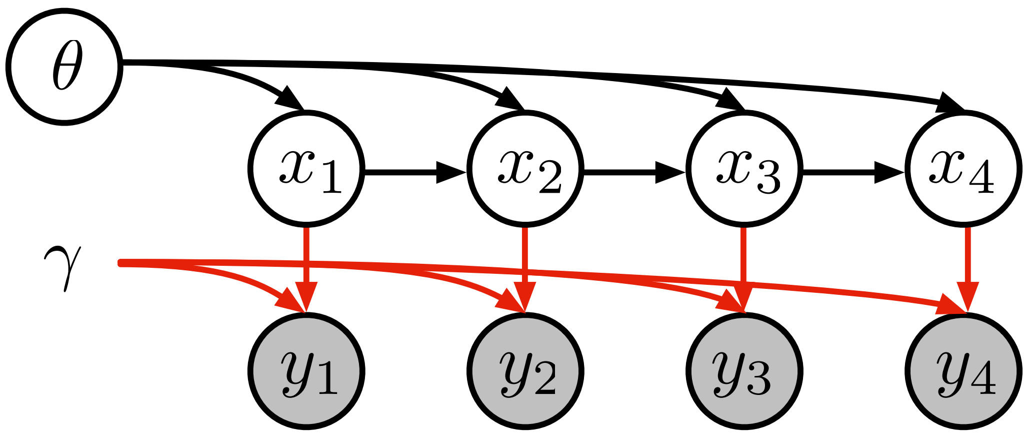


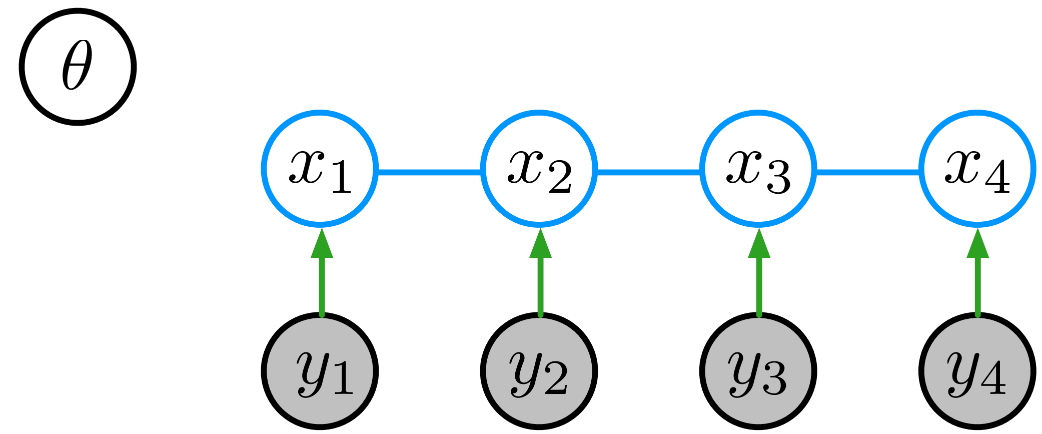






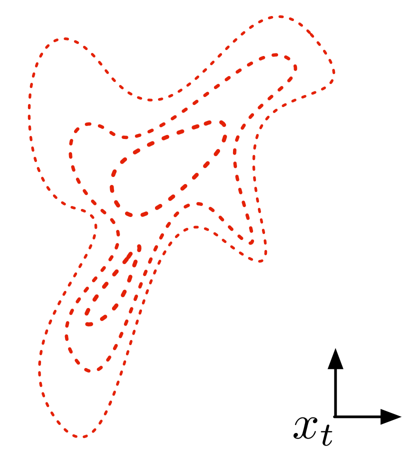
$$\mathcal{L}(\eta_\theta, \eta_x) \triangleq \mathbb{E}_{q(\theta)q(x)}\left[\log \frac{p(\theta, x)p(y \mid x, \gamma)}{q(\theta)q(x)}\right]$$

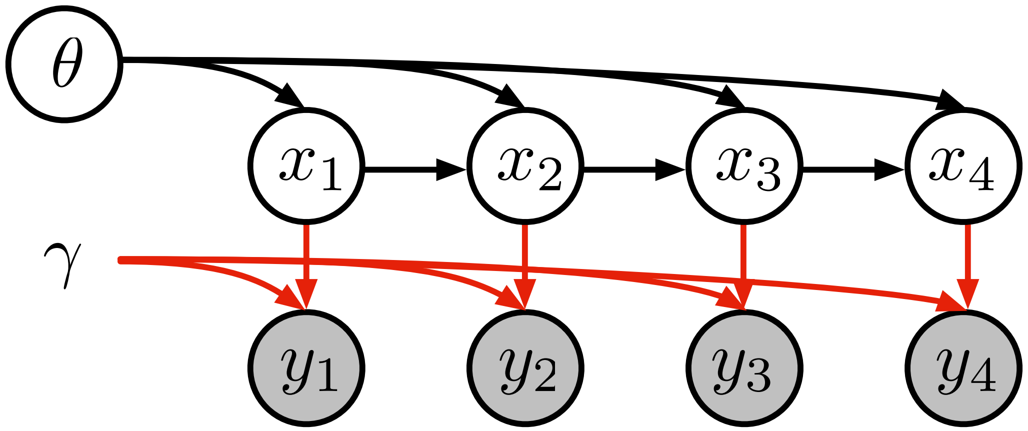


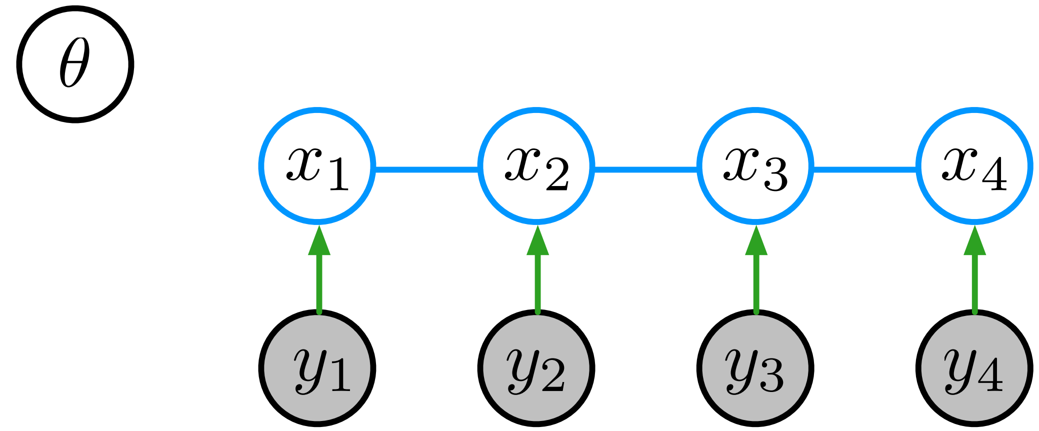


$$\mathbb{E}_{q(\gamma)} \log p(y_t \mid x_t, \gamma)$$

$$\mathcal{L}(\eta_\theta, \eta_x) \triangleq \mathbb{E}_{q(\theta)q(x)}\left[\log \frac{p(\theta, x)p(y \mid x, \gamma)}{q(\theta)q(x)}\right]$$

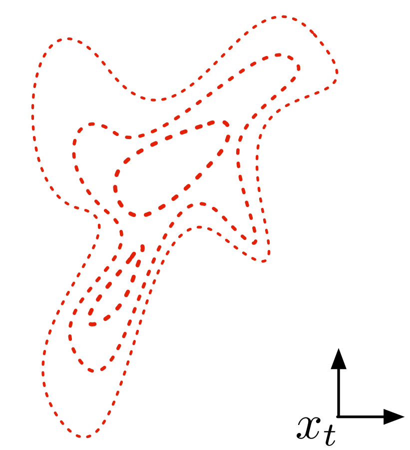






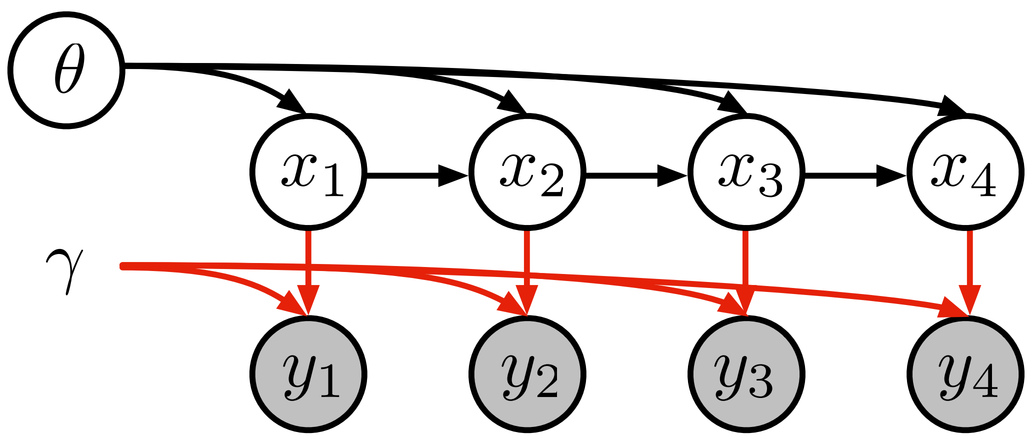
$$\mathcal{L}(\eta_\theta, \eta_x) \triangleq \mathbb{E}_{q(\theta)q(x)}\left[\log \frac{p(\theta, x)p(y \,|\, x, \gamma)}{q(\theta)q(x)}\right]$$

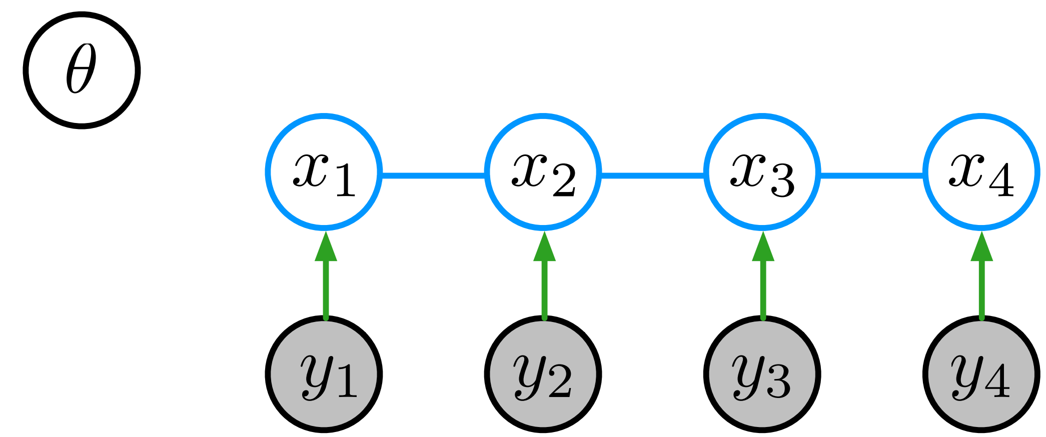
$$\mathbb{E}_{q(\gamma)} \log p(y_t \,|\, x_t, \gamma)$$



$$\widehat{\mathcal{L}}(\eta_\theta, \eta_x, \phi) \triangleq \mathbb{E}_{q(\theta)q(x)}\left[\log \frac{p(\theta, x)\exp(\psi(x\,;\, y, \phi))}{q(\theta)q(x)}\right]$$

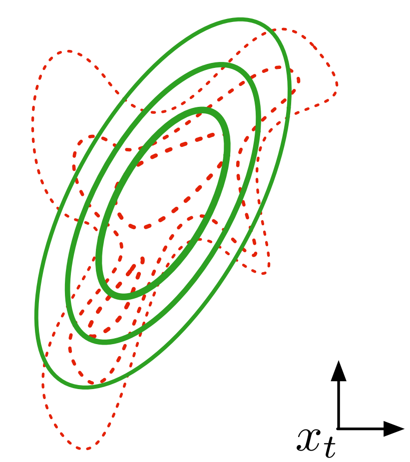
where $\psi(x\,;\, y, \phi)$ is a conjugate potential for $p(x \,|\, \theta)$.





$$\mathcal{L}(\eta_\theta, \eta_x) \triangleq \mathbb{E}_{q(\theta)q(x)}\left[\log \frac{p(\theta, x)p(y \mid x, \gamma)}{q(\theta)q(x)}\right]$$

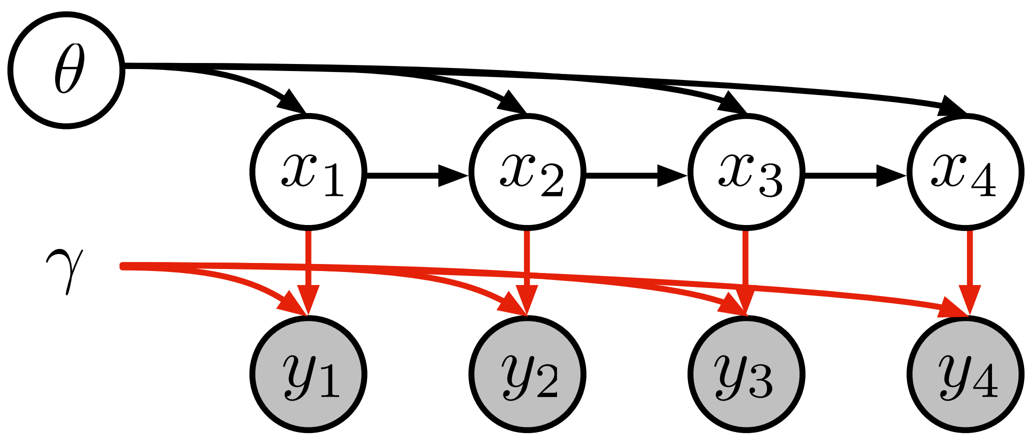
$\mathbb{E}_{q(\gamma)} \log p(y_t \mid x_t, \gamma)$

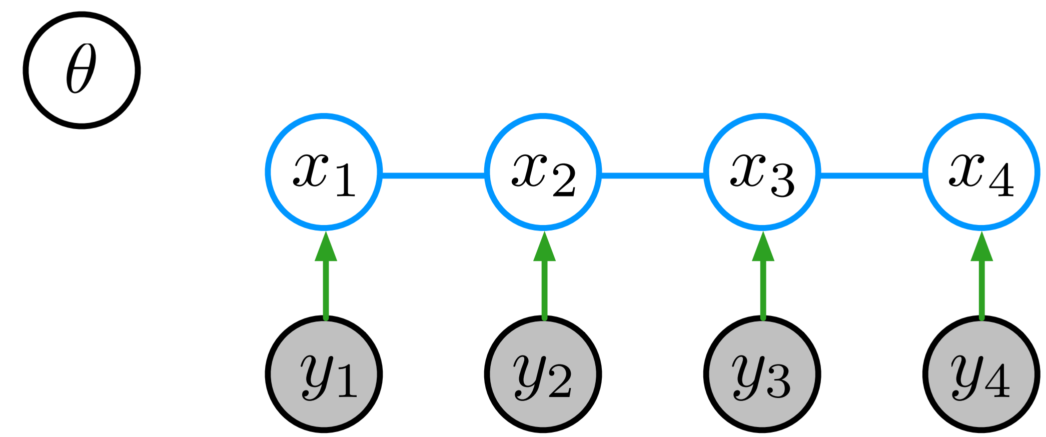


$\psi(x_t; y_t, \phi)$

$$\widehat{\mathcal{L}}(\eta_\theta, \eta_x, \phi) \triangleq \mathbb{E}_{q(\theta)q(x)}\left[\log \frac{p(\theta, x)\exp(\psi(x\,;\,y, \phi))}{q(\theta)q(x)}\right]$$

where $\psi(x\,;\,y, \phi)$ is a conjugate potential for $p(x \mid \theta)$.





$$\mathcal{L}(\eta_\theta, \eta_x) \triangleq \mathbb{E}_{q(\theta)q(x)}\left[\log \frac{p(\theta, x)p(y \,|\, x, \gamma)}{q(\theta)q(x)}\right]$$

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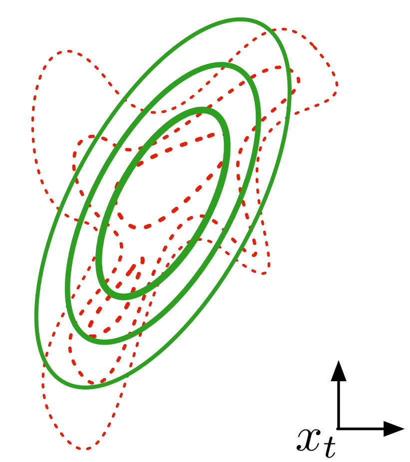

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where $\psi(x\,;\,y, \phi)$ is a conjugate potential for $p(x \,|\, \theta)$.

$$\eta_x^*(\eta_\theta, \phi) \triangleq \arg\max_{\eta_x} \widehat{\mathcal{L}}(\eta_\theta, \eta_x, \phi) \qquad \mathcal{L}_{\text{SVAE}}(\eta_\theta, \phi) \triangleq \mathcal{L}(\eta_\theta, \eta_x^*(\eta_\theta, \phi))$$

Step 1: apply recognition network

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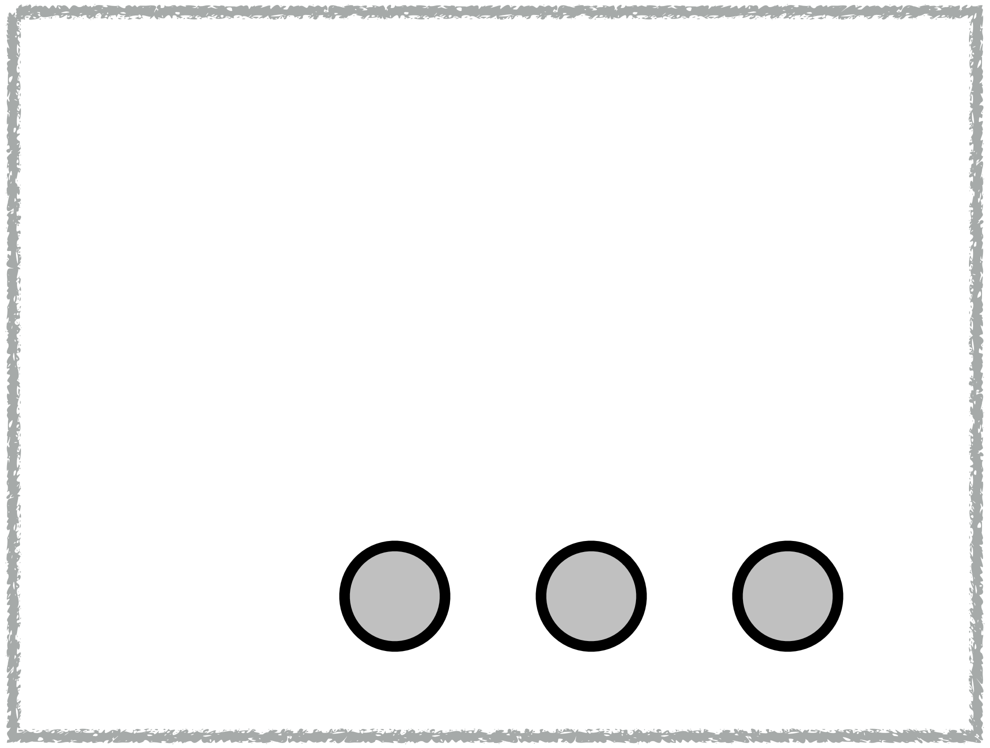

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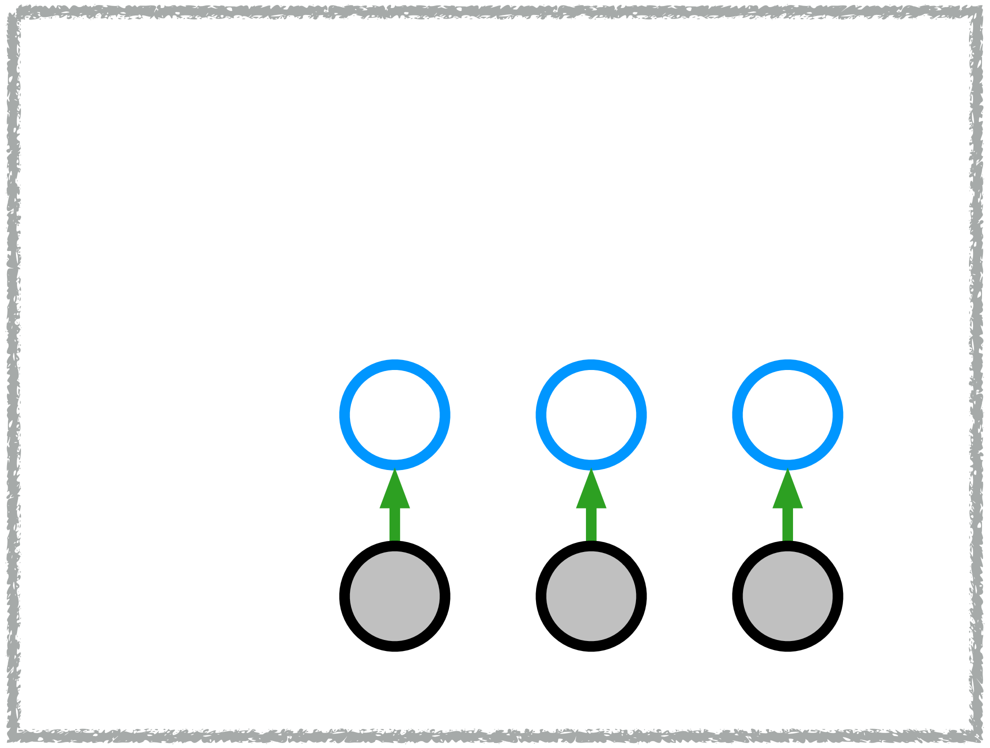

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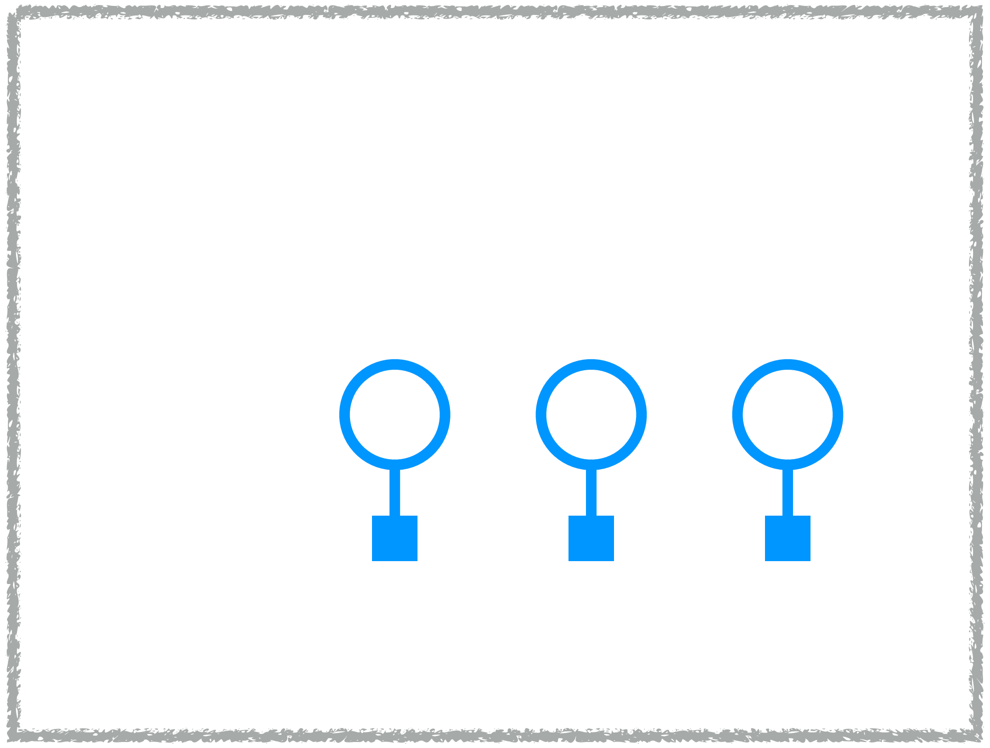

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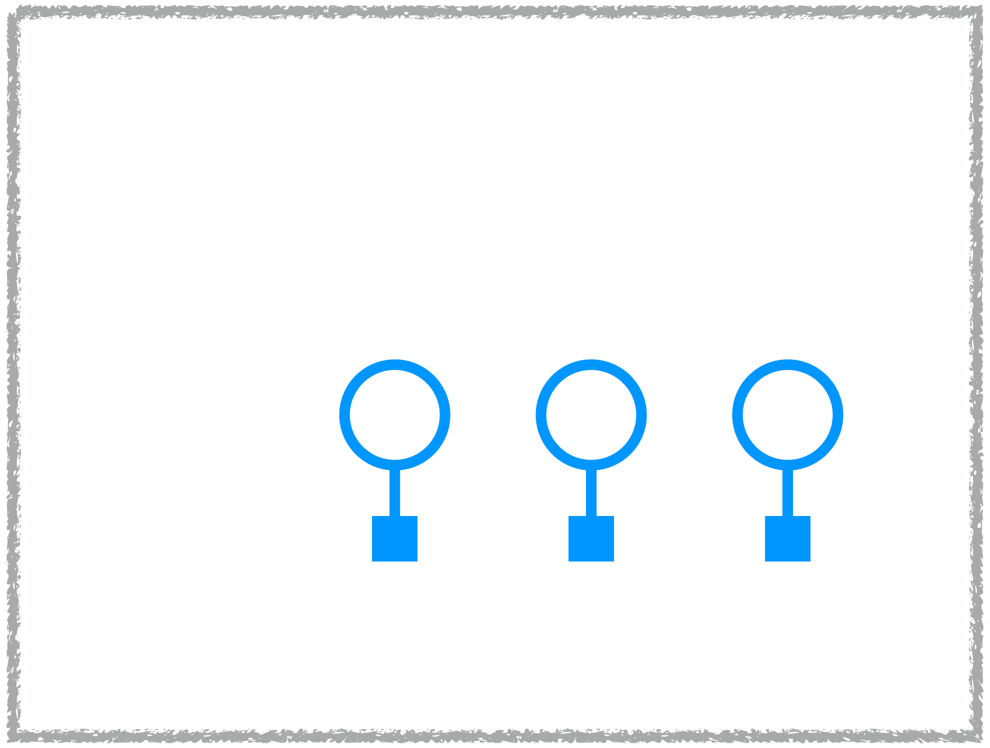
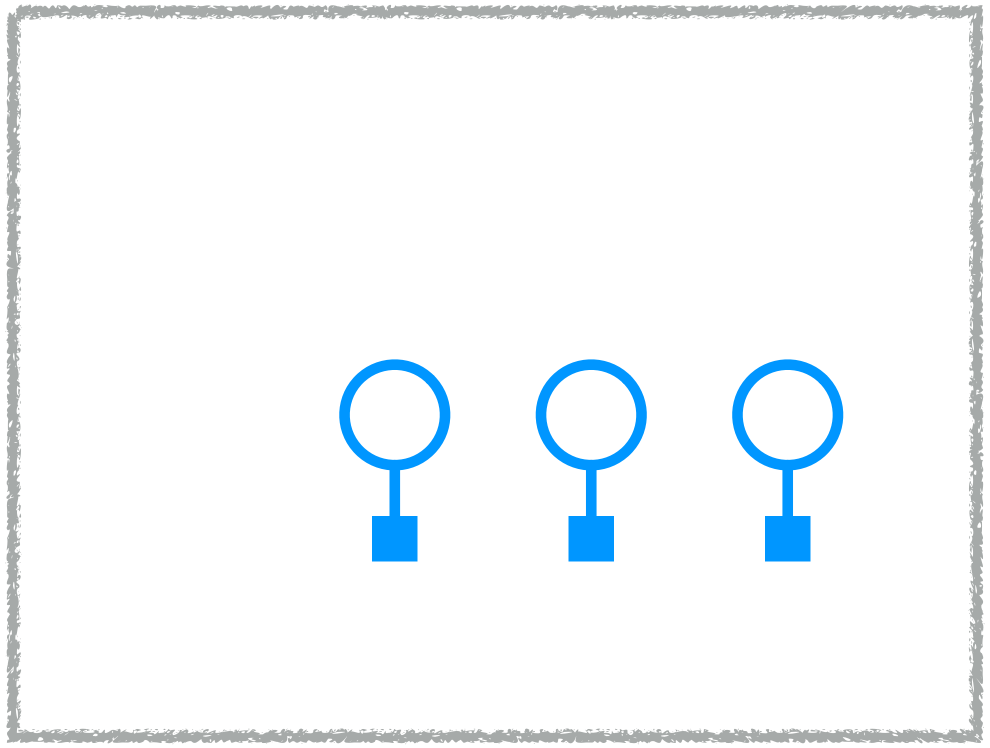


Step 2: run fast PGM algorithms

Step 1: apply recognition network



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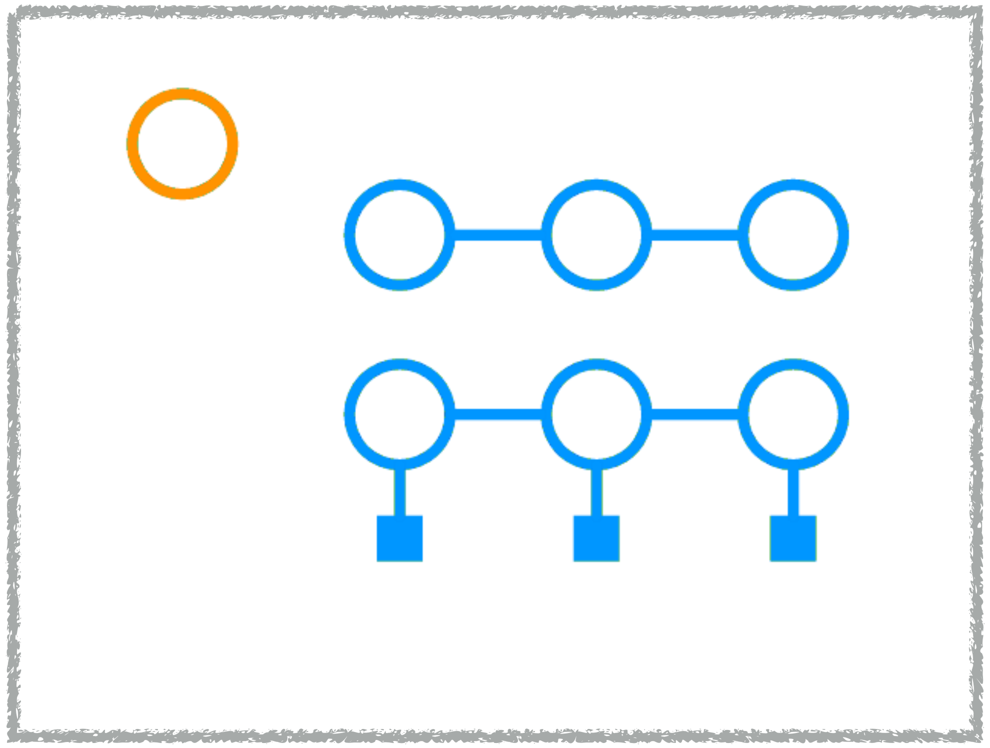

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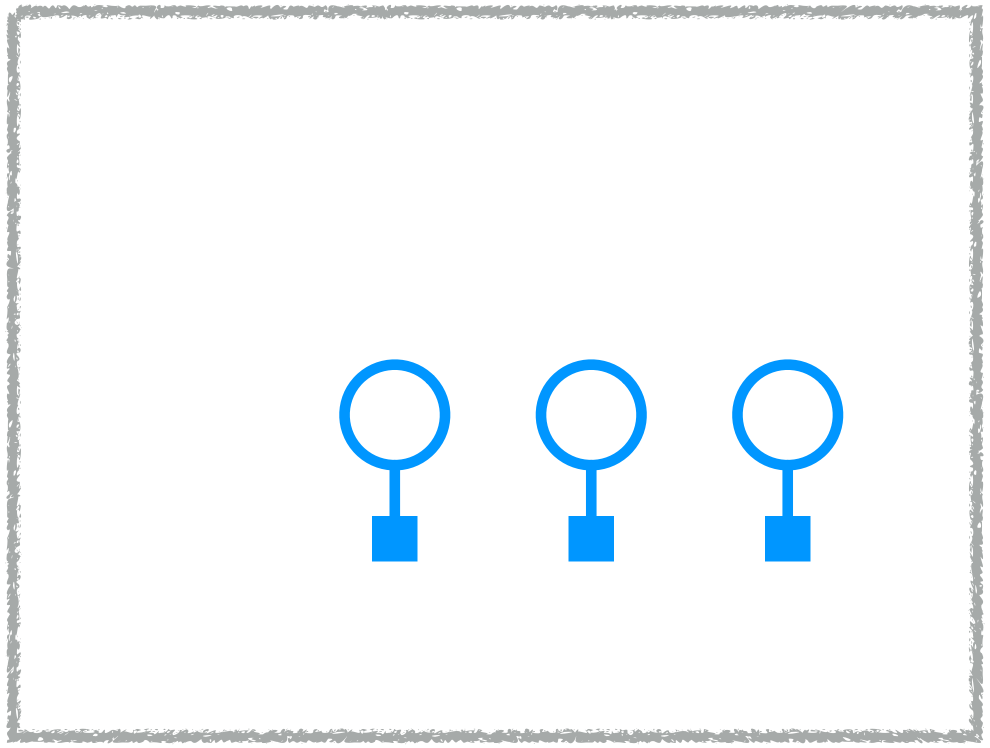

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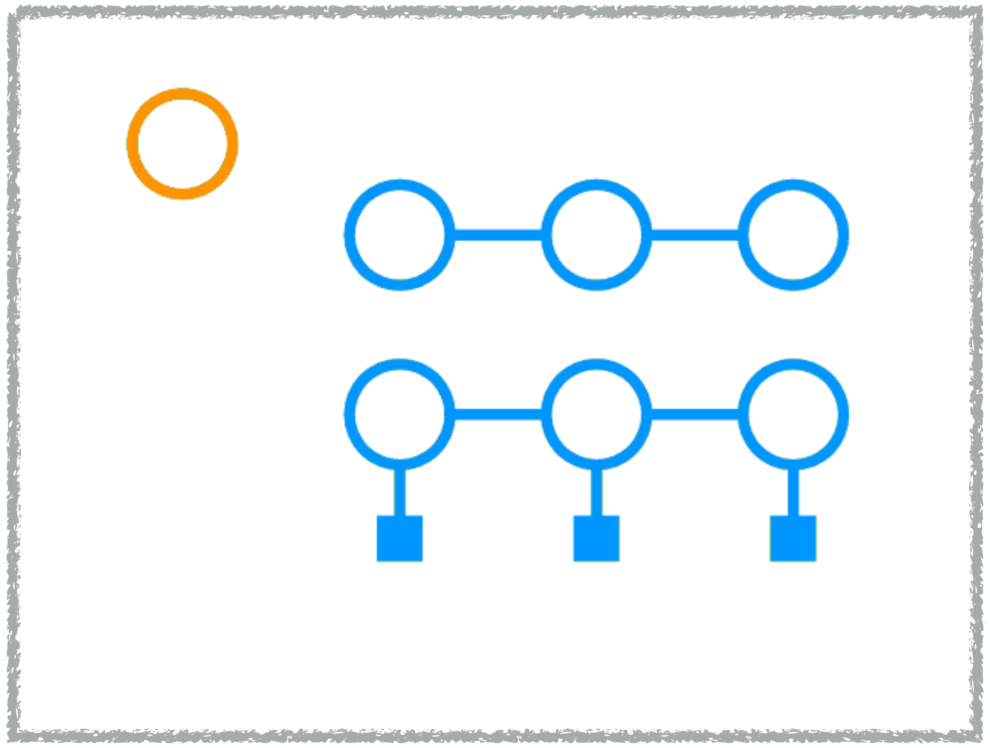
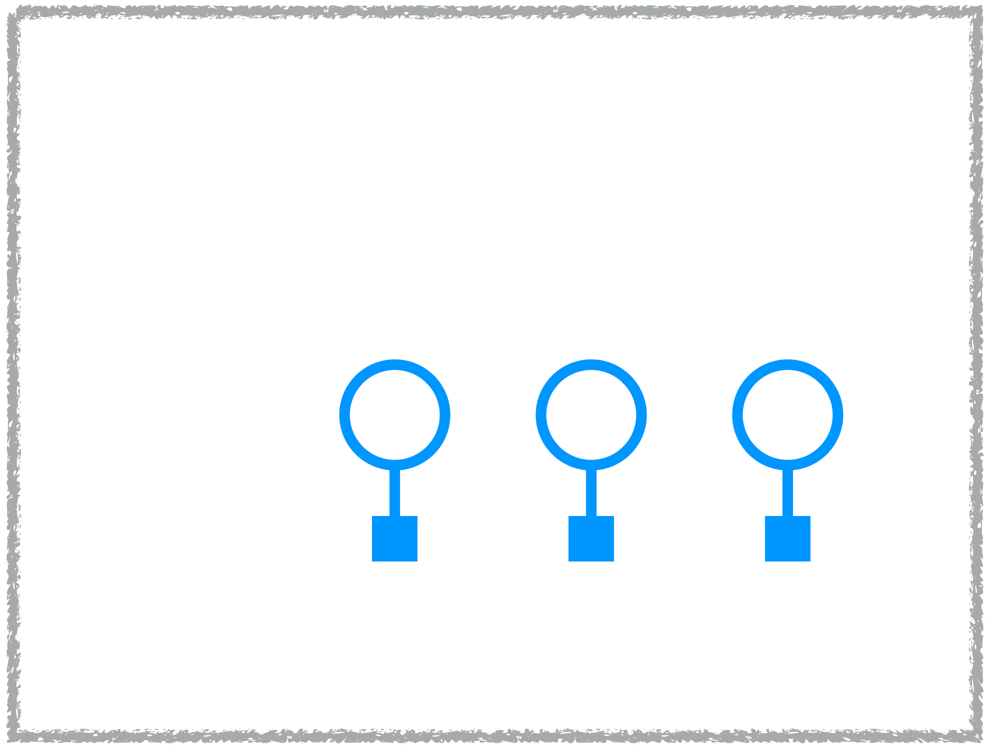


Step 3: sample, compute flat grads

Step 1: apply recognition network



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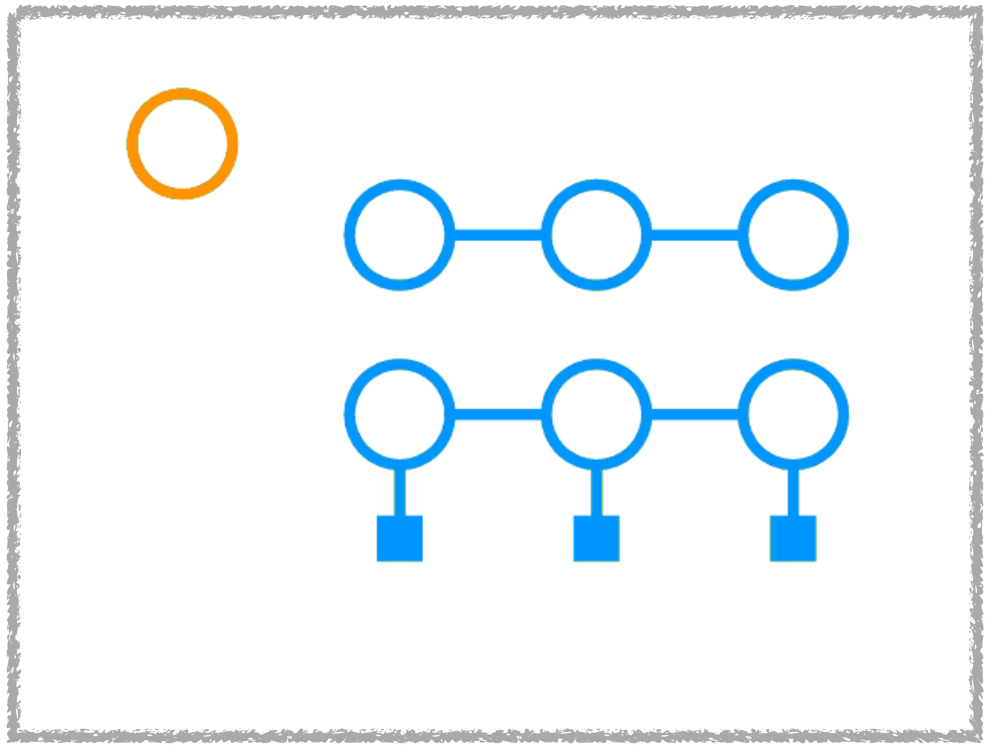

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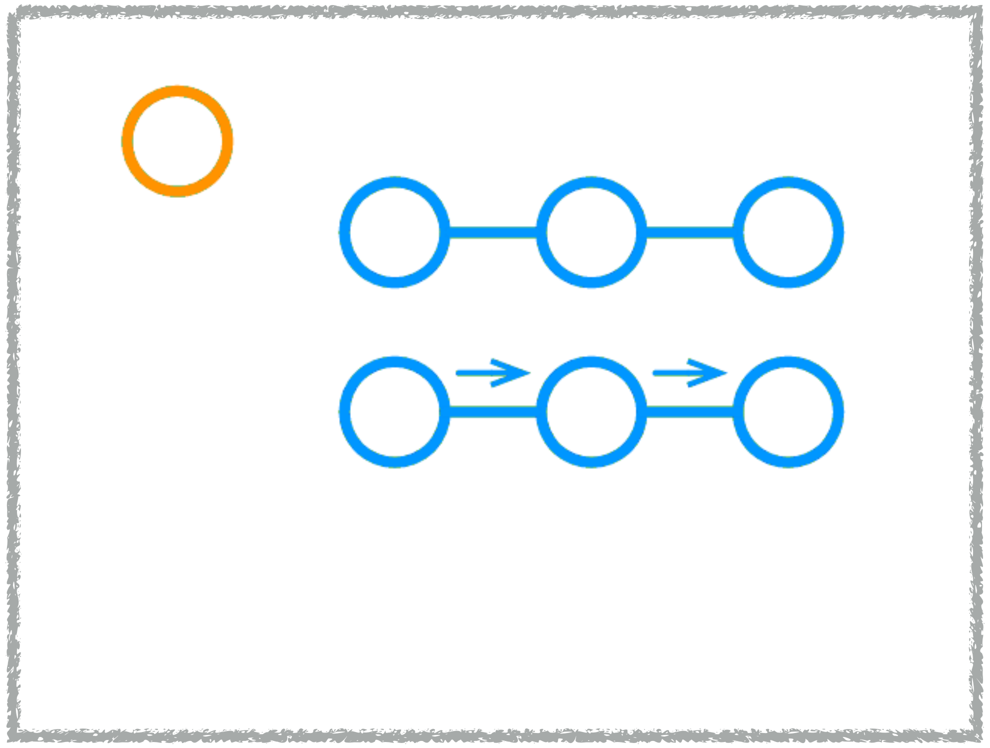
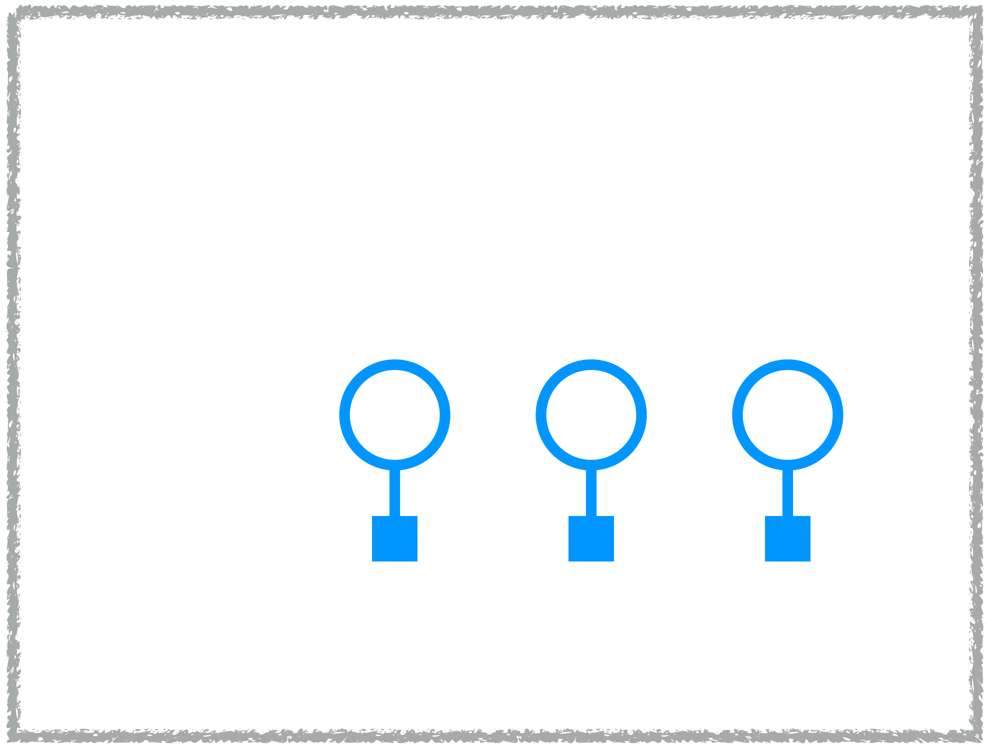


Step 1: apply recognition network



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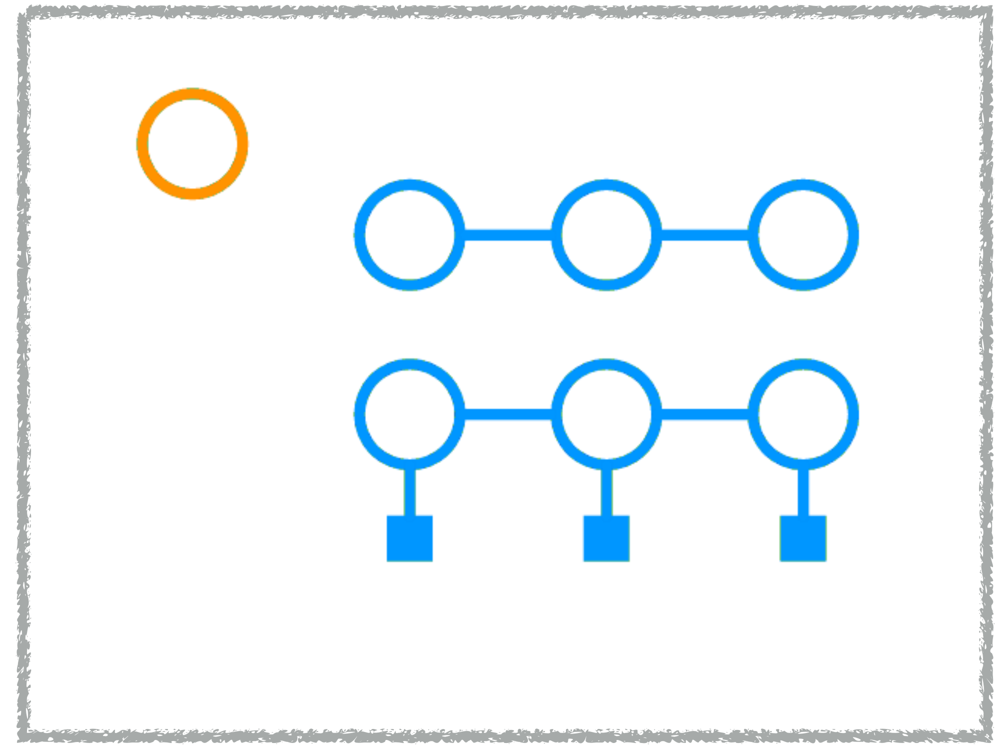
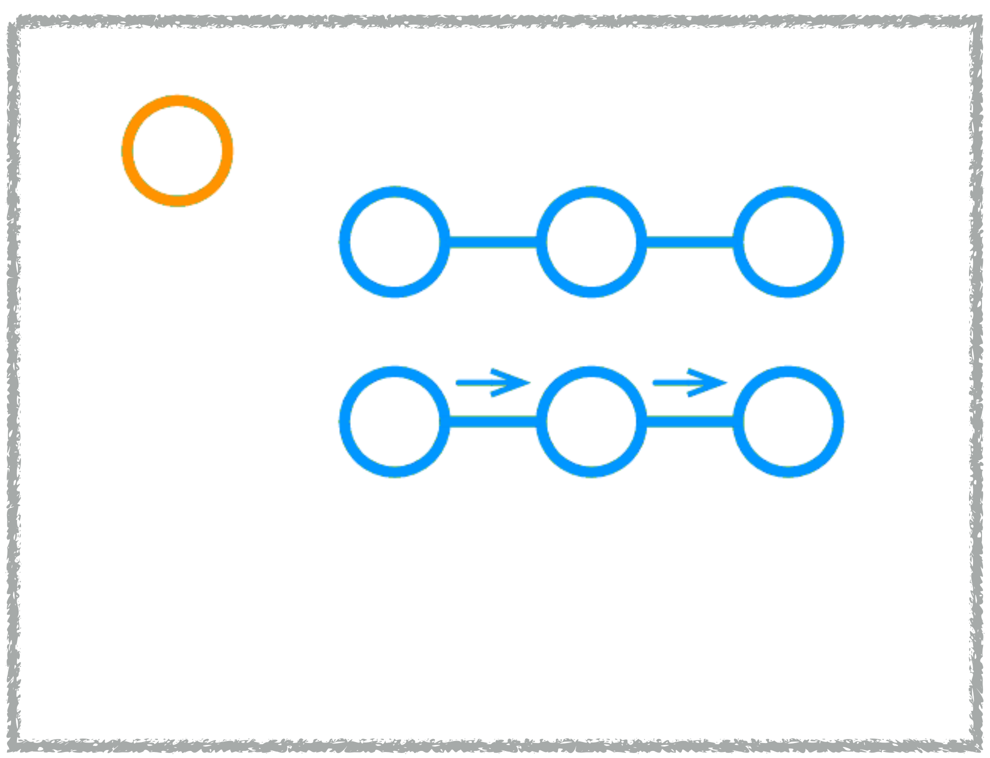
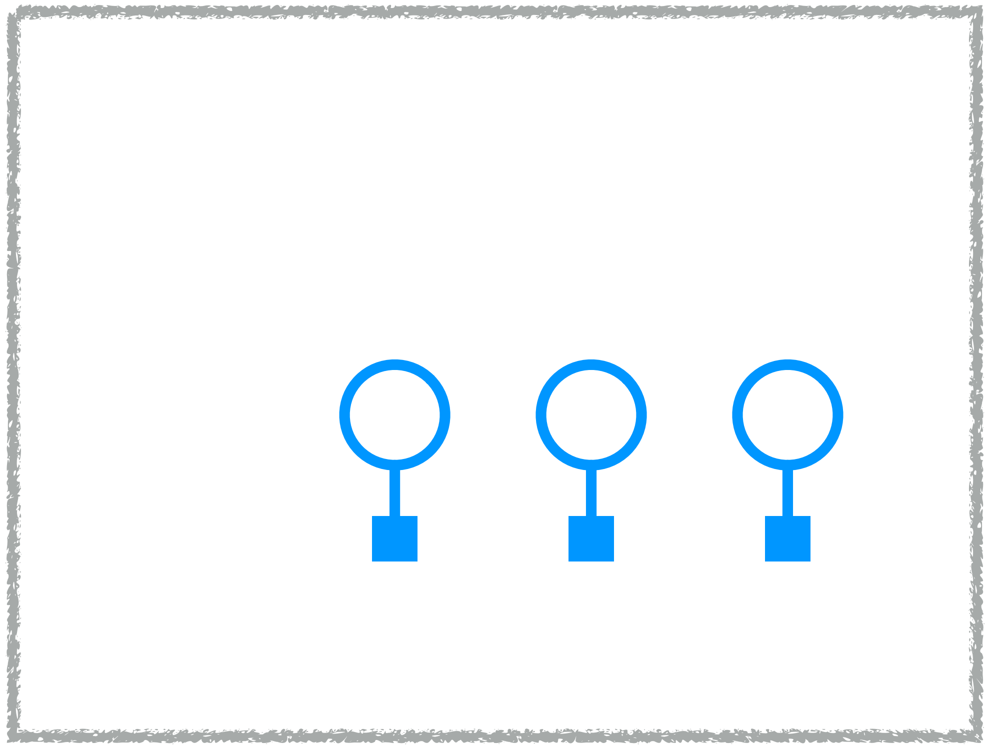


Step 3: sample, compute flat grads

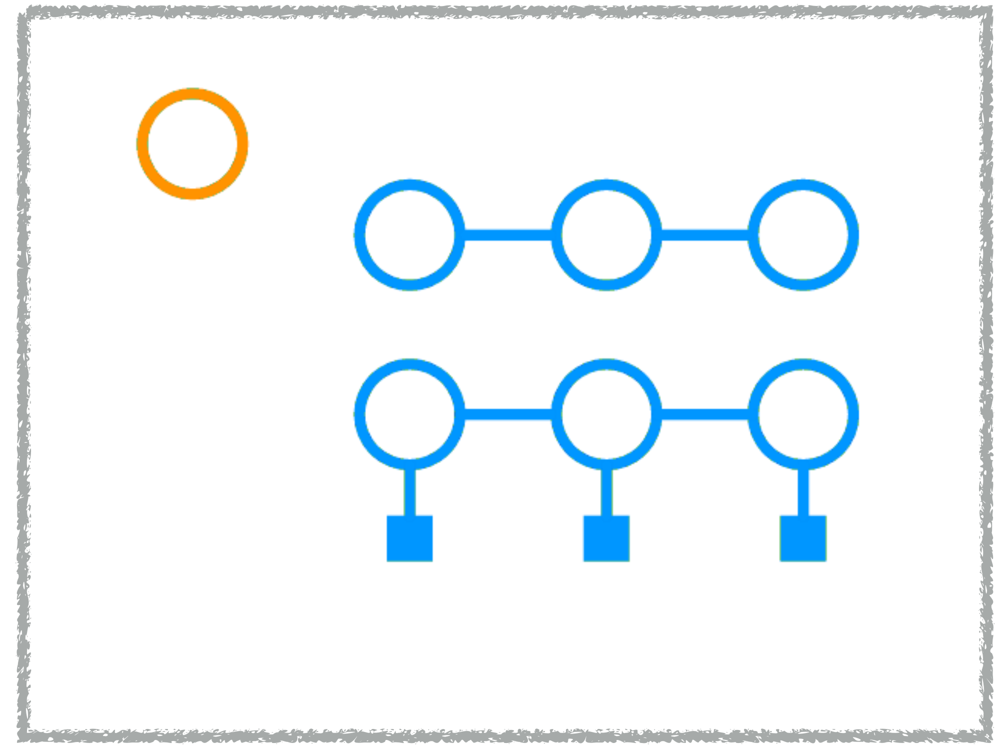


Step 4: compute natural gradient

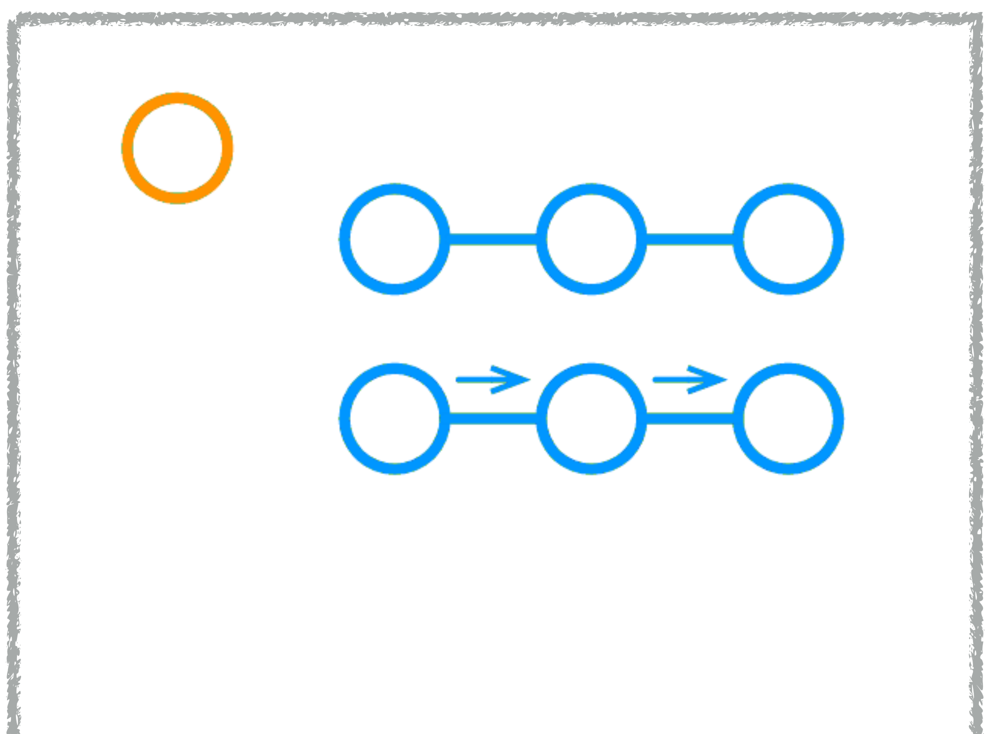
Step 1: apply recognition network



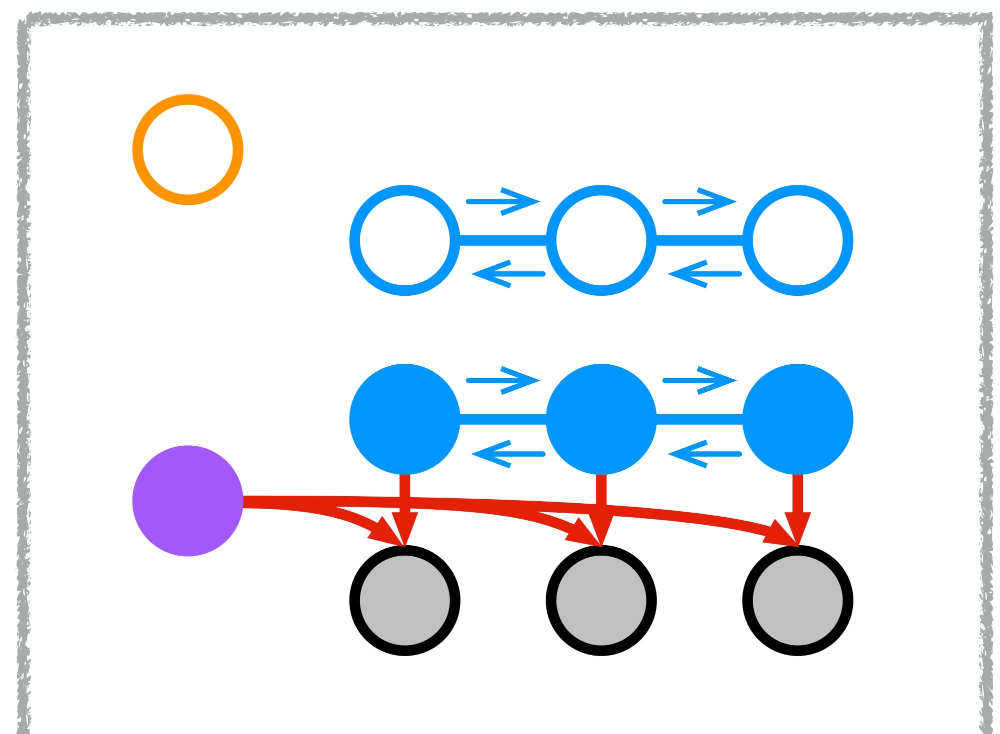
Step 2: run fast PGM algorithms

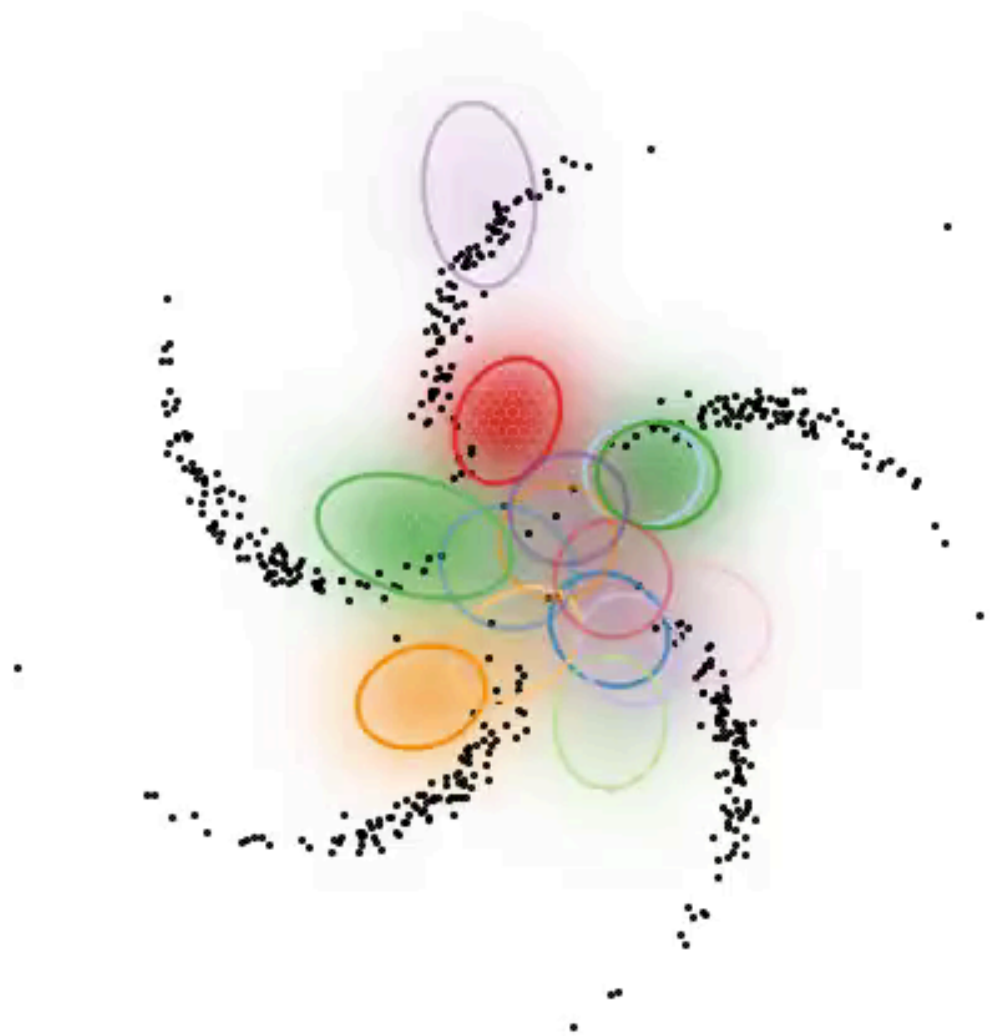


Step 3: sample, compute flat grads

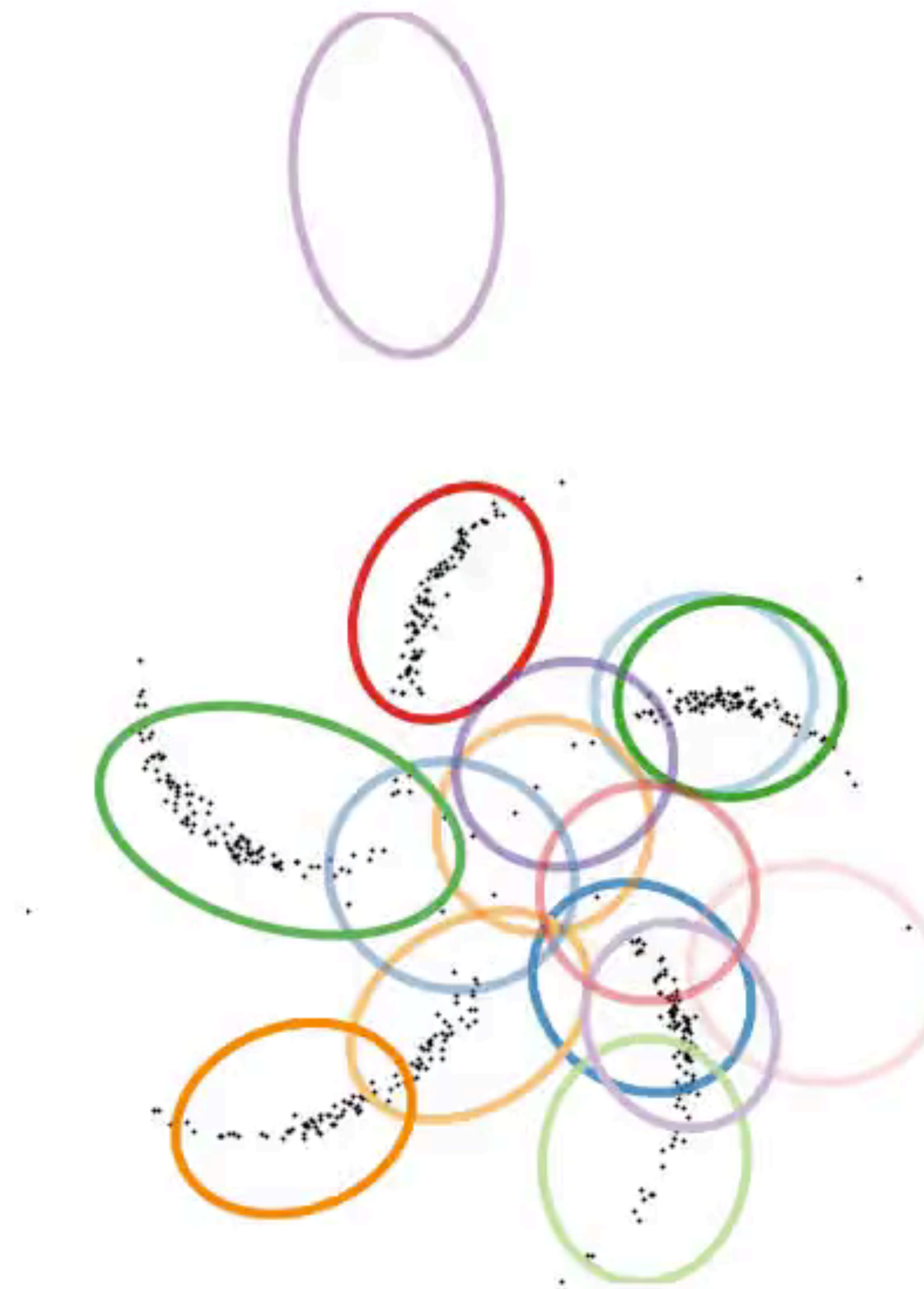


Step 4: compute natural gradient

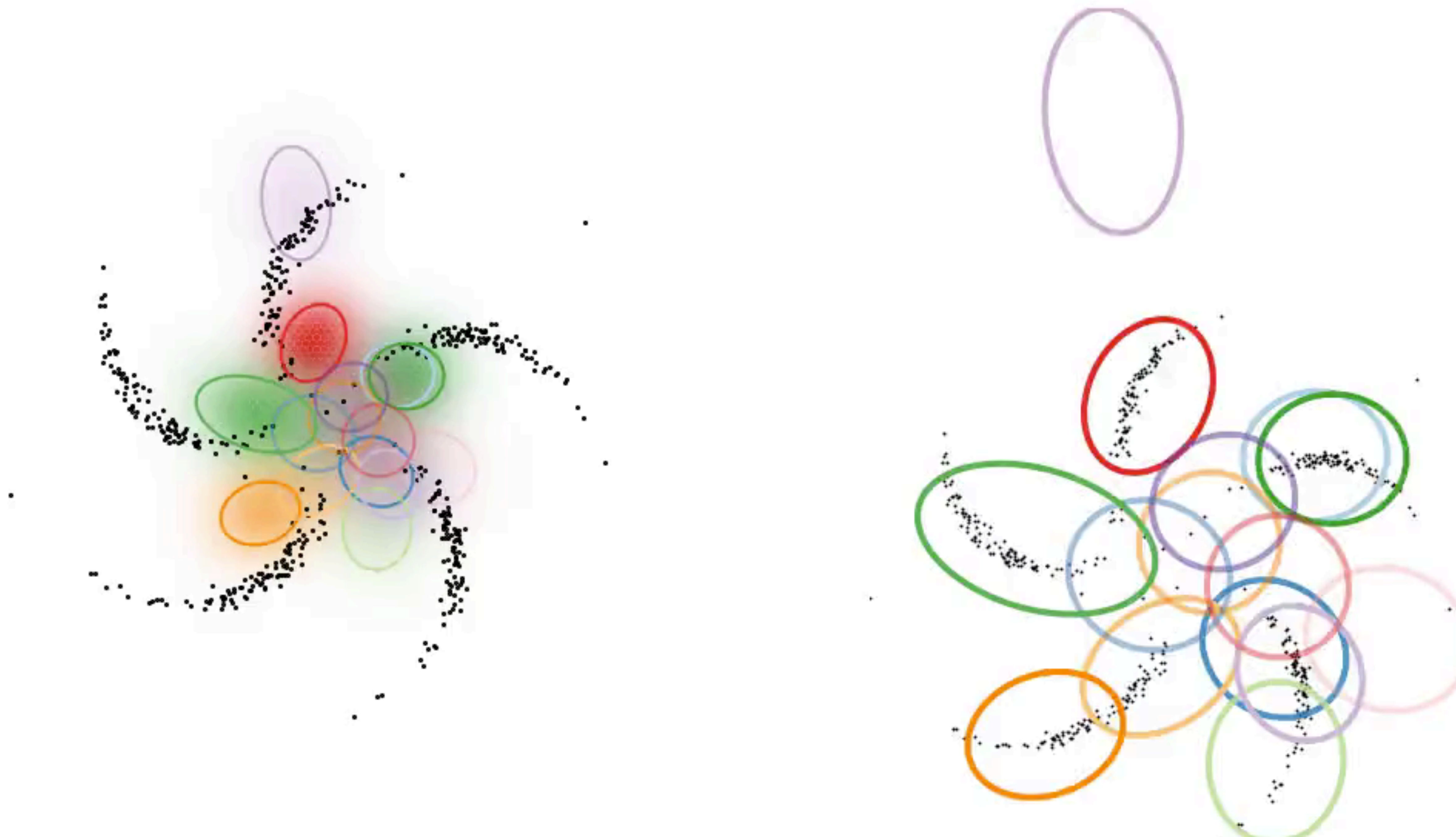




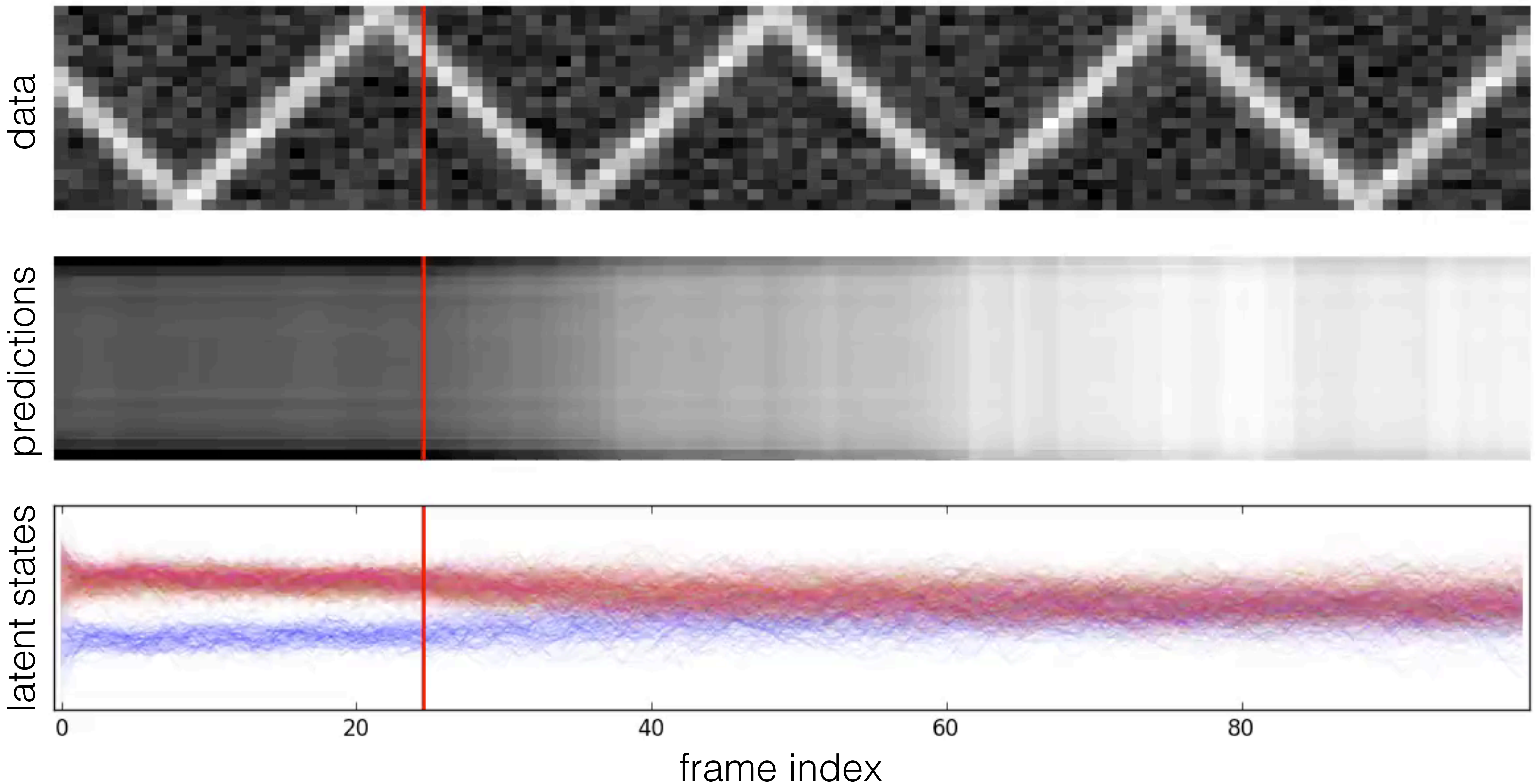
data space



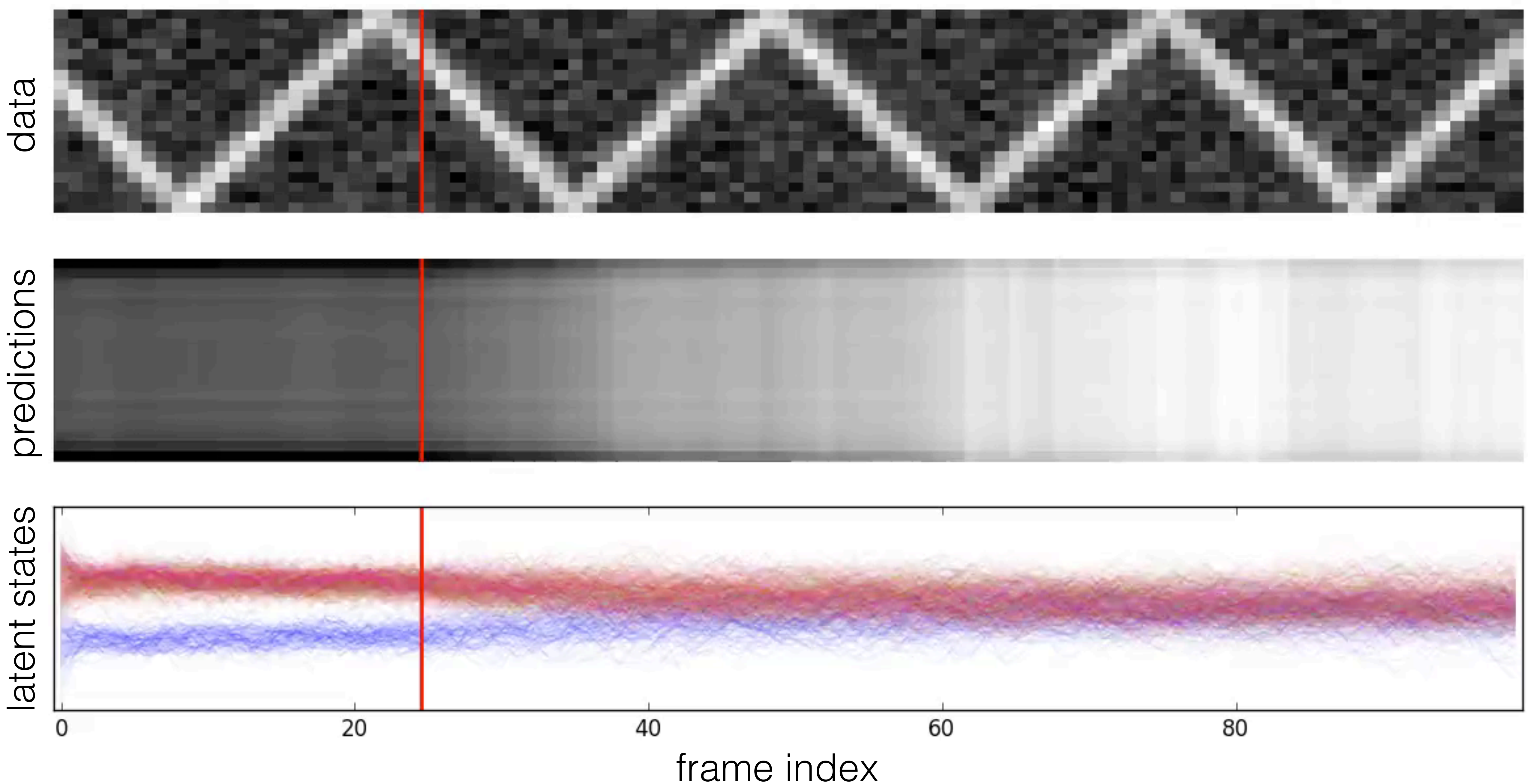
latent space



data space latent space



data
predictions
latent states
0
20
40
60
80
frame index


data
predictions
latent states
0
20
40
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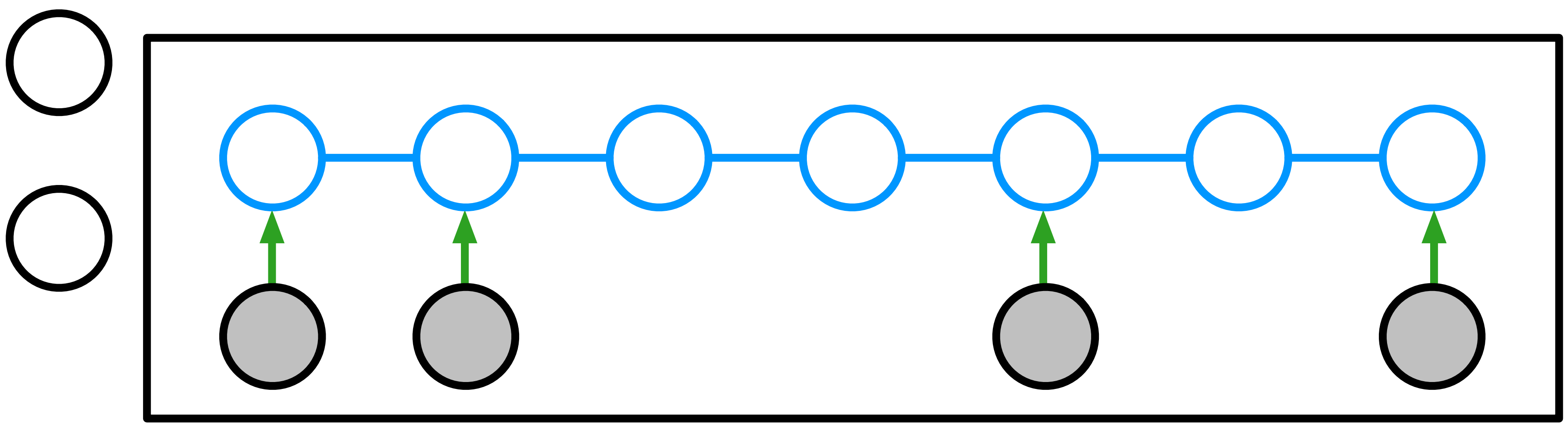
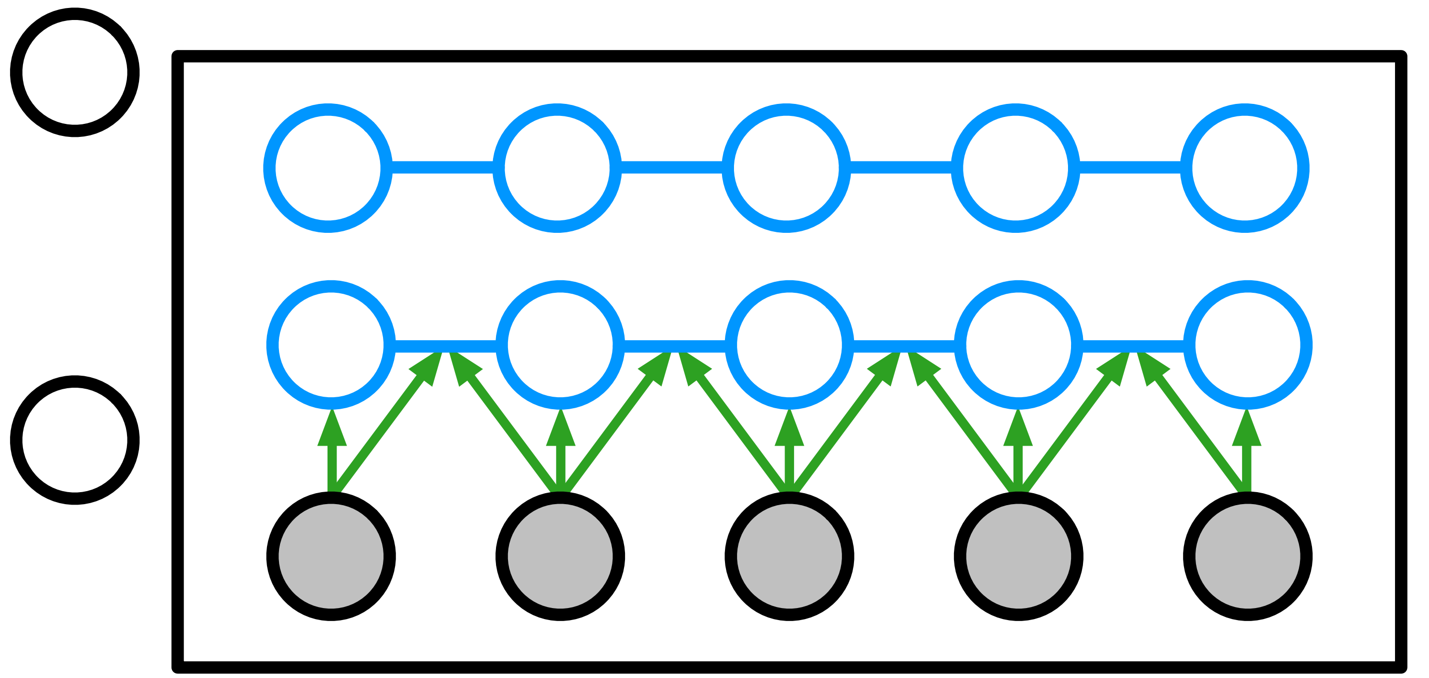
80
frame index

arbitrary inference queries*

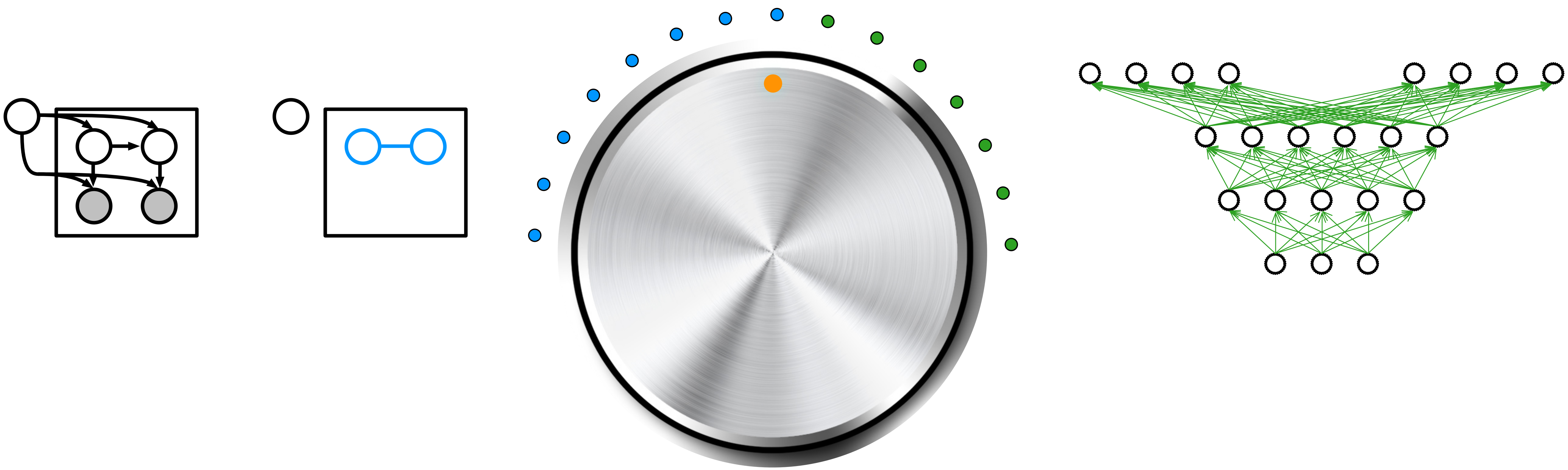


*see next slide

SVAEs can use any inference network architectures

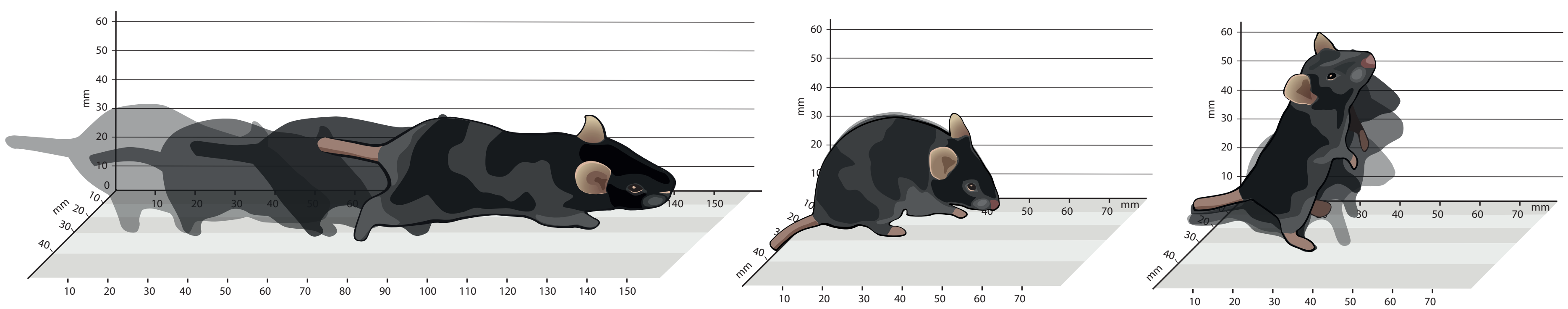


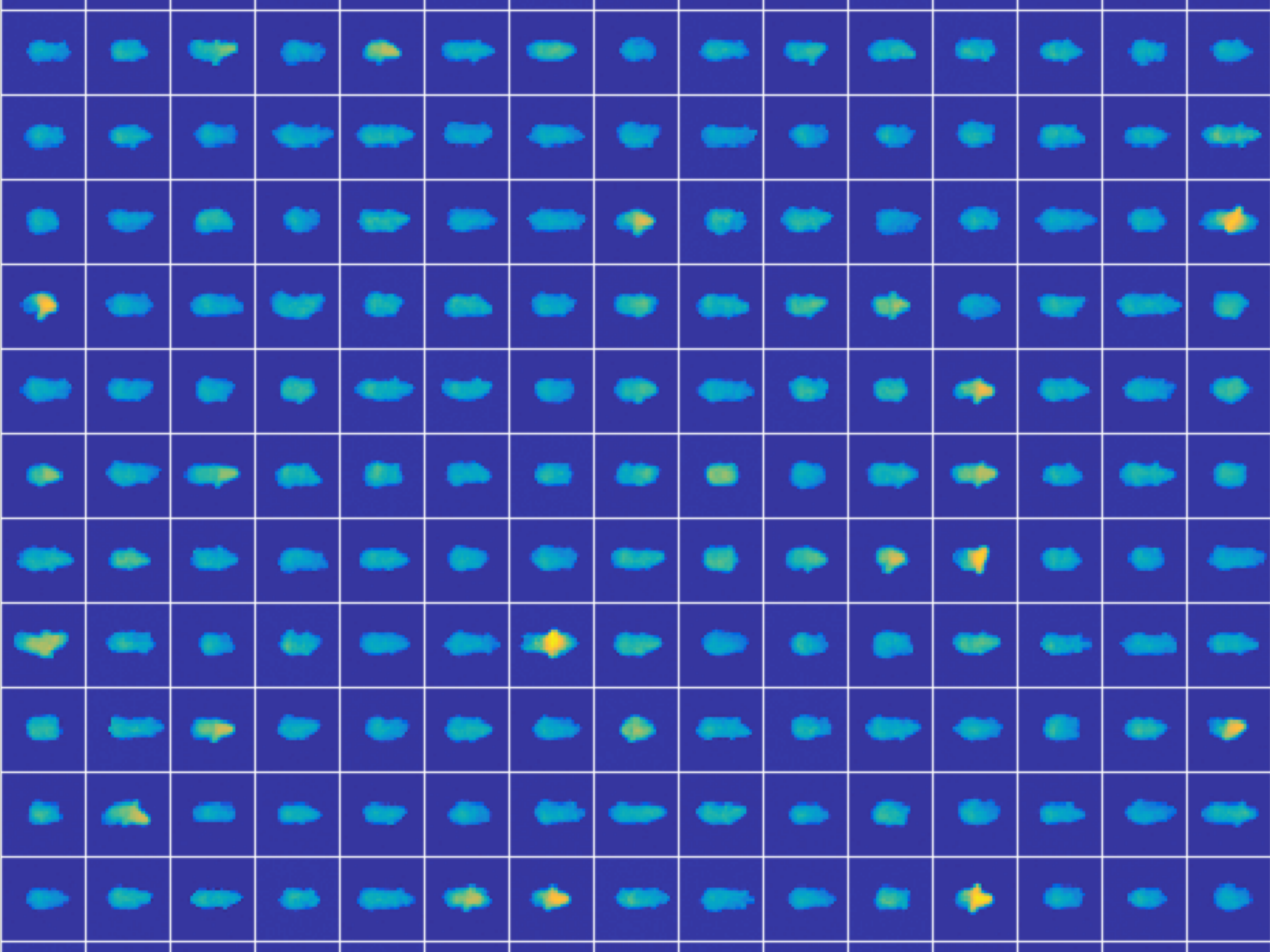
[1] Archer, Park, Buesing, Cunningham, Paninski. Black box variational inference for state space models. ICLR 2016 Workshops.
[2] Gao*, Archer*, Paninski, Cunningham. Linear dynamical neural population models through nonlinear embeddings. NIPS 2016.

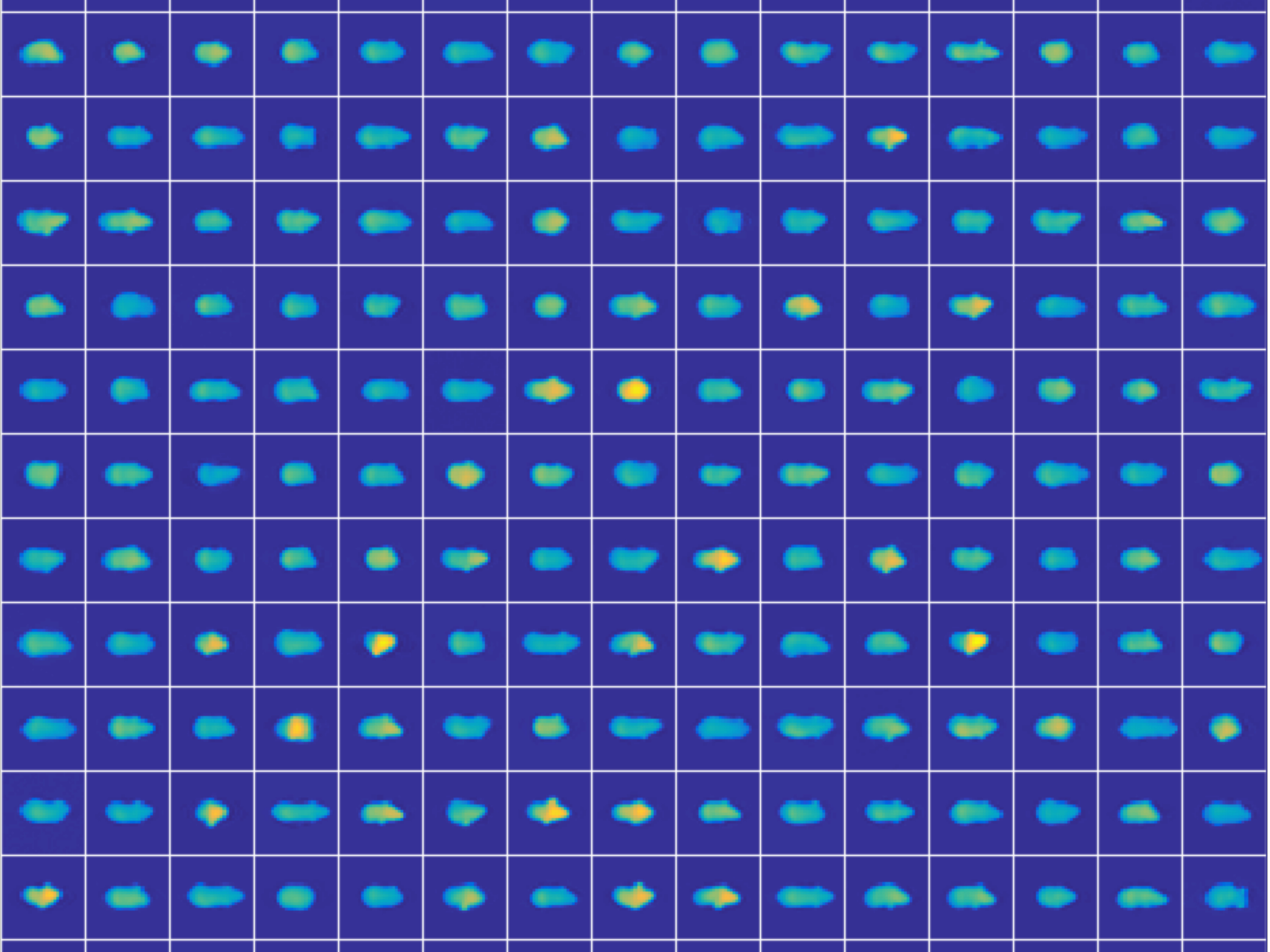


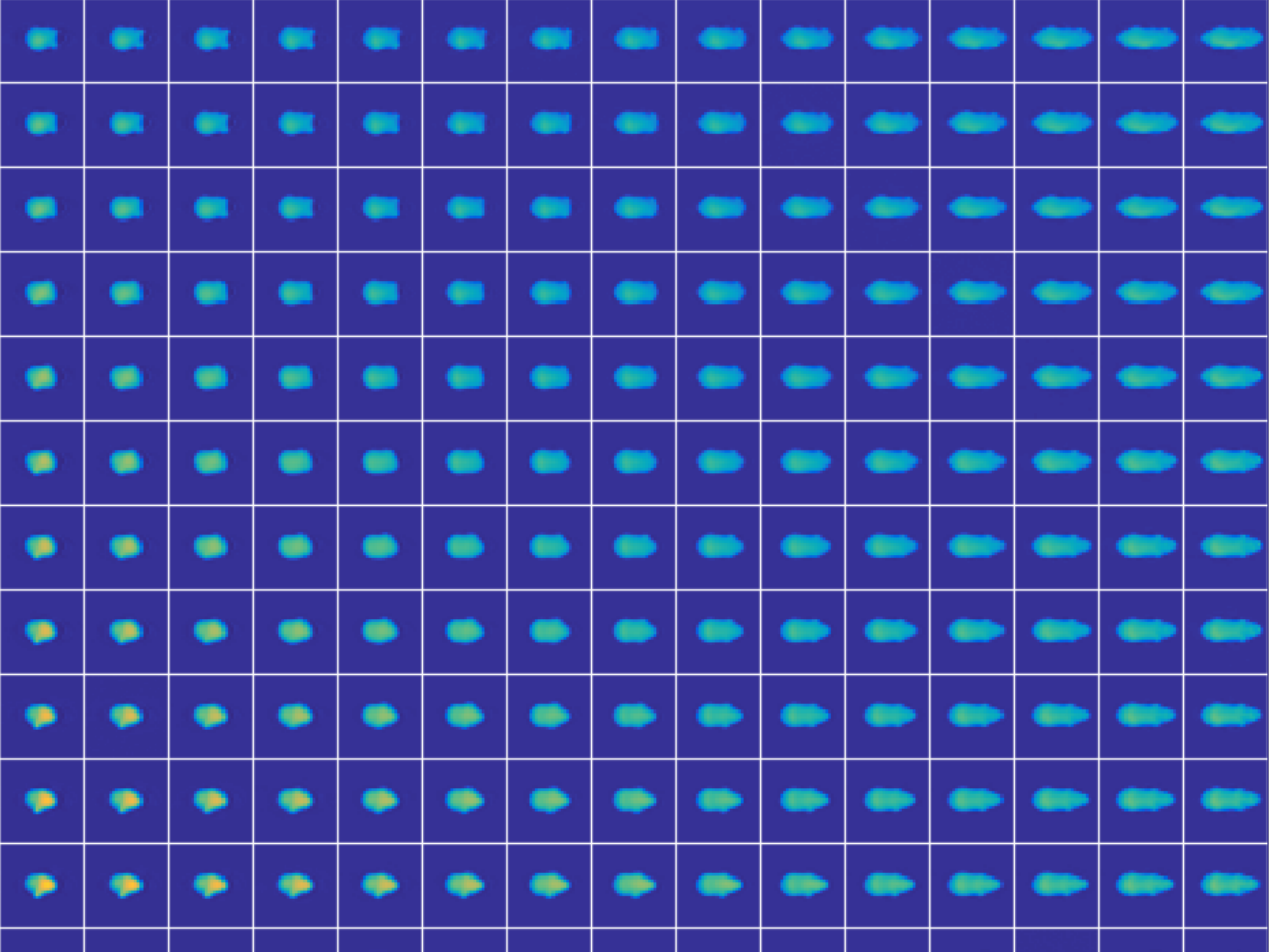
SVAEs

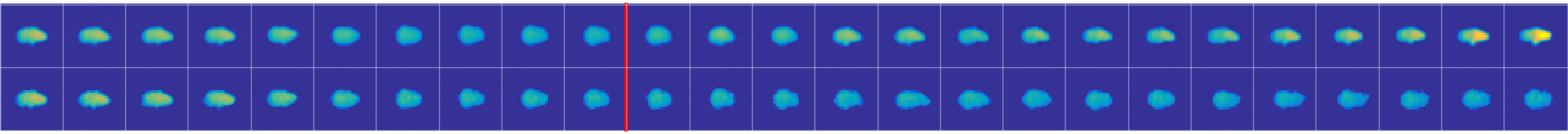
Application: learn syllable representation of behavior from video

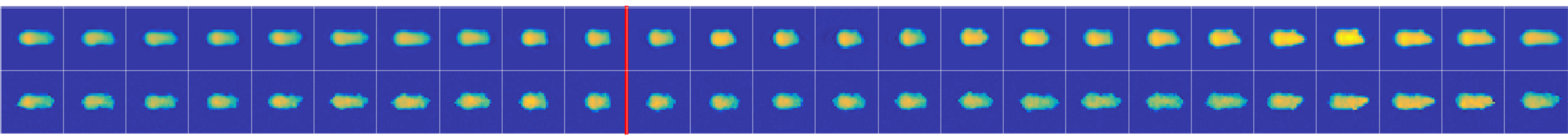


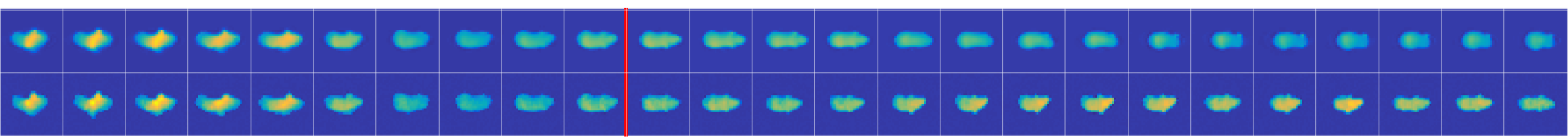


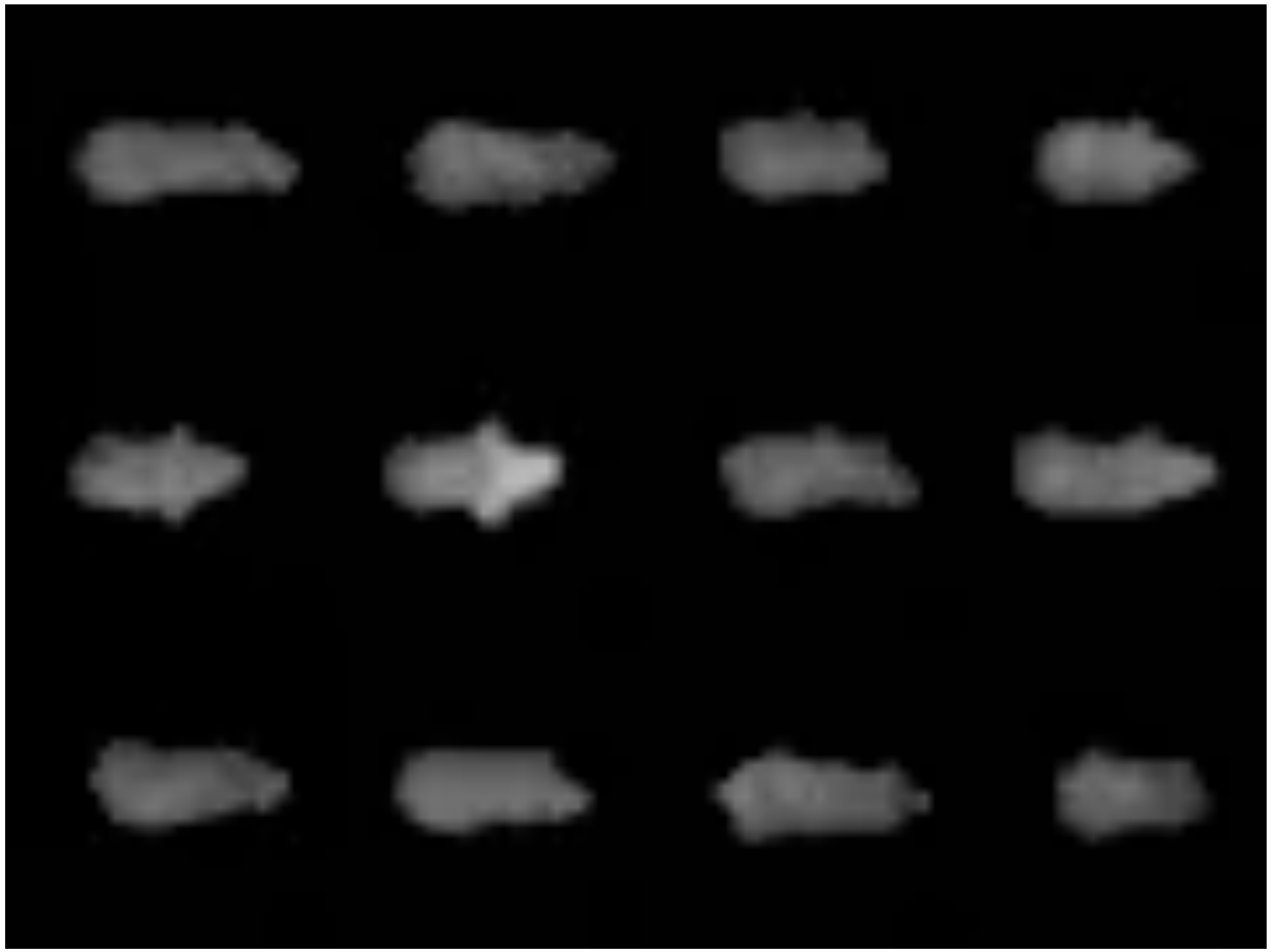




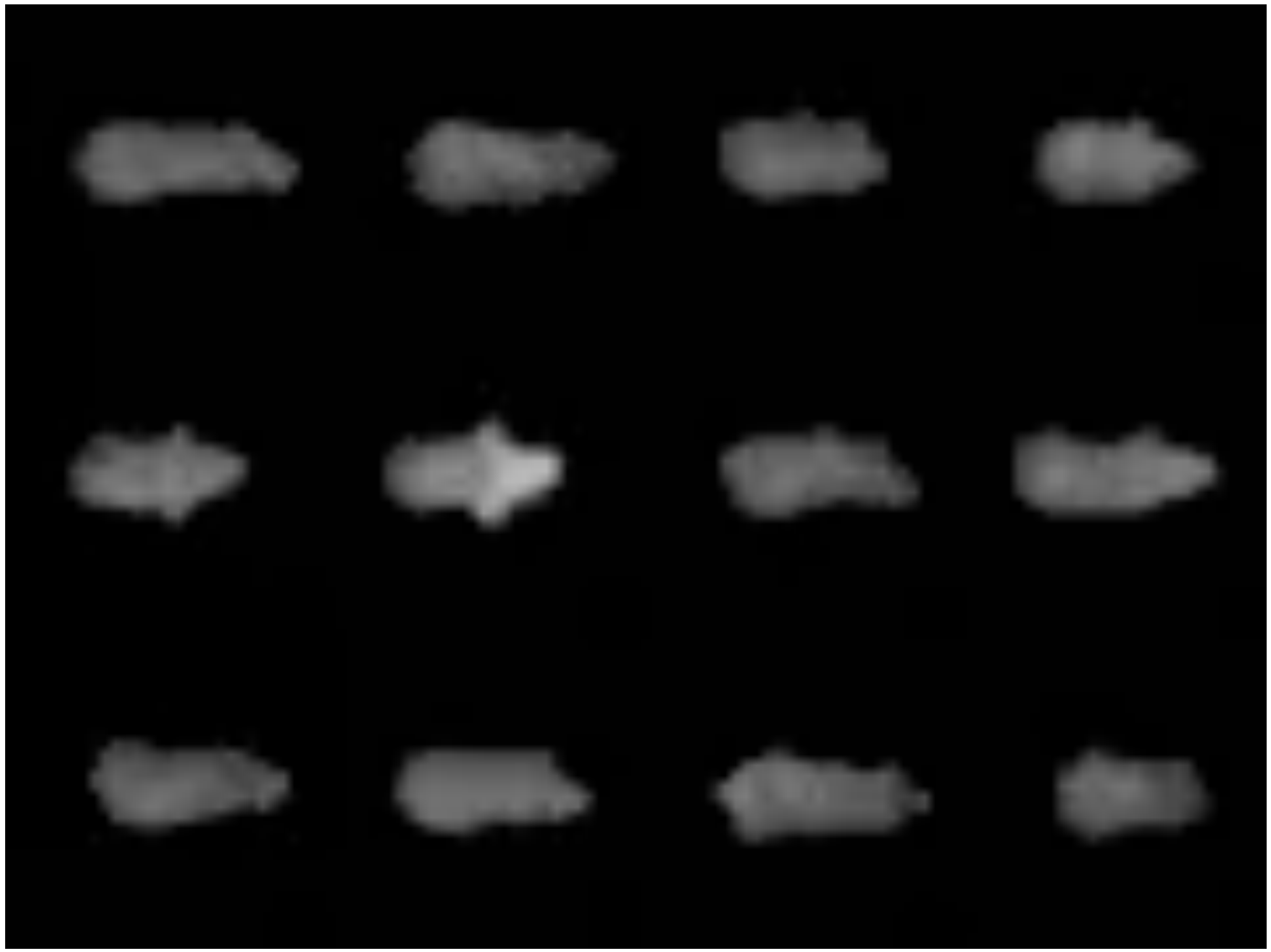








start rear



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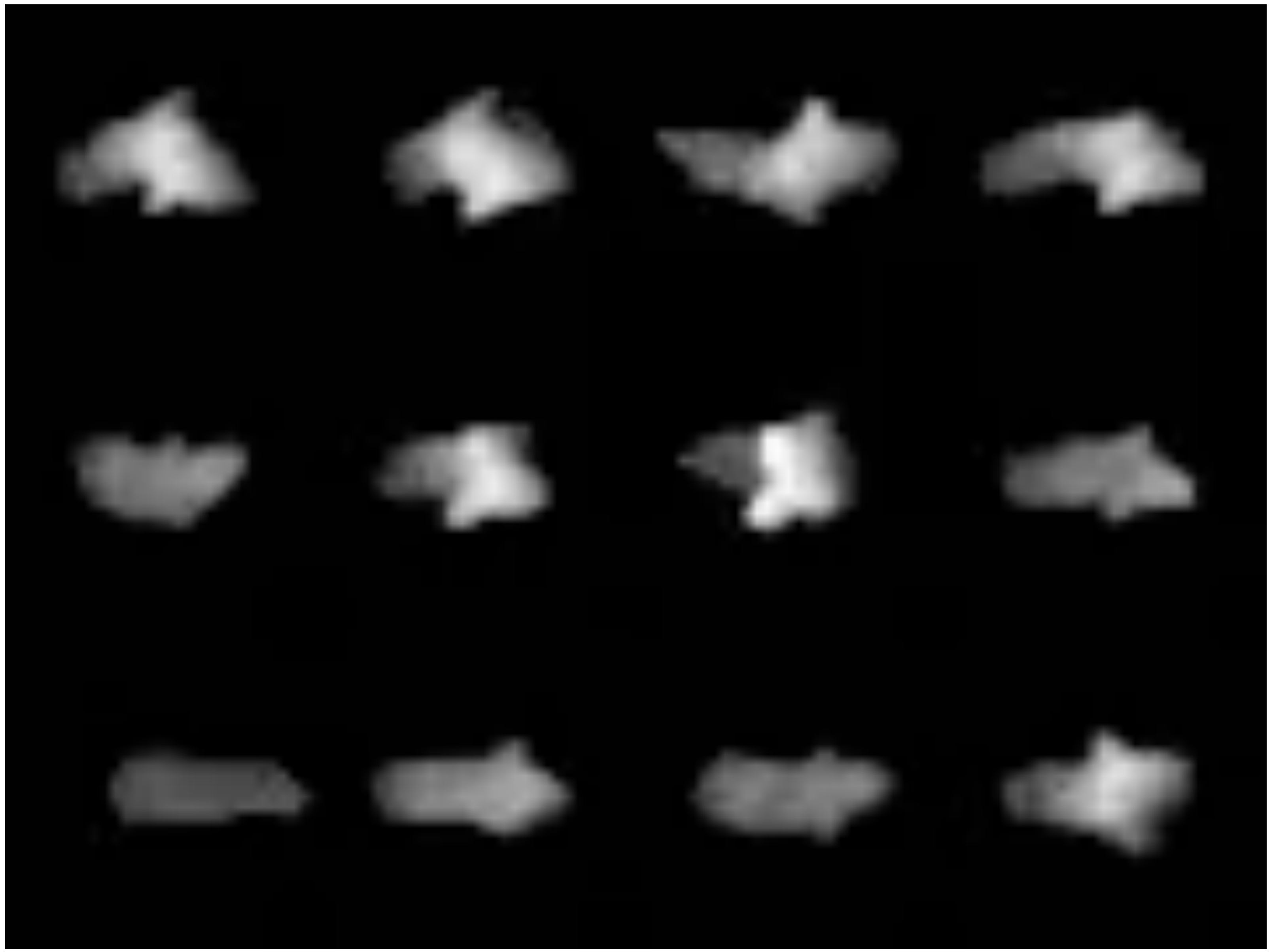
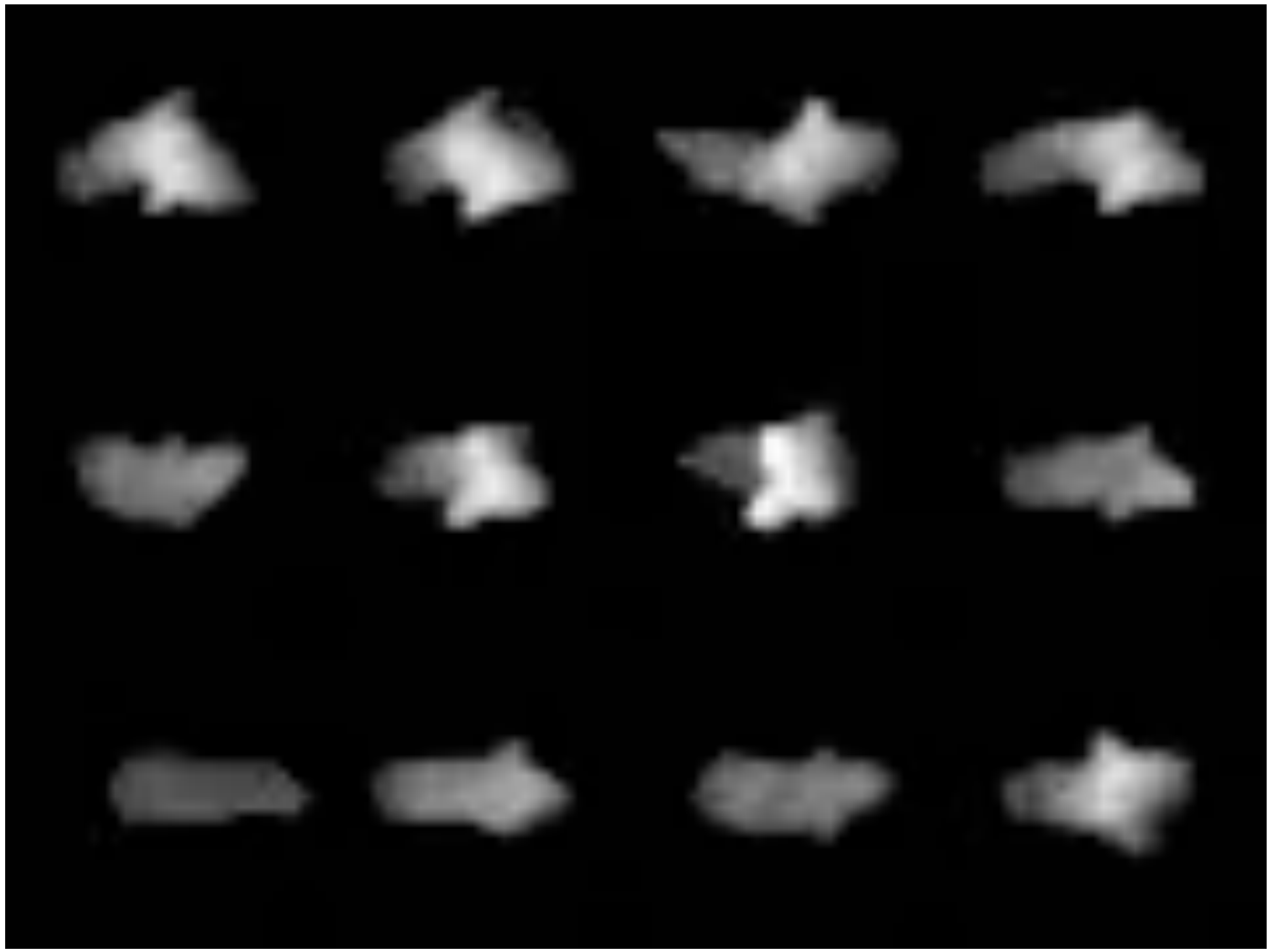


fall from rear



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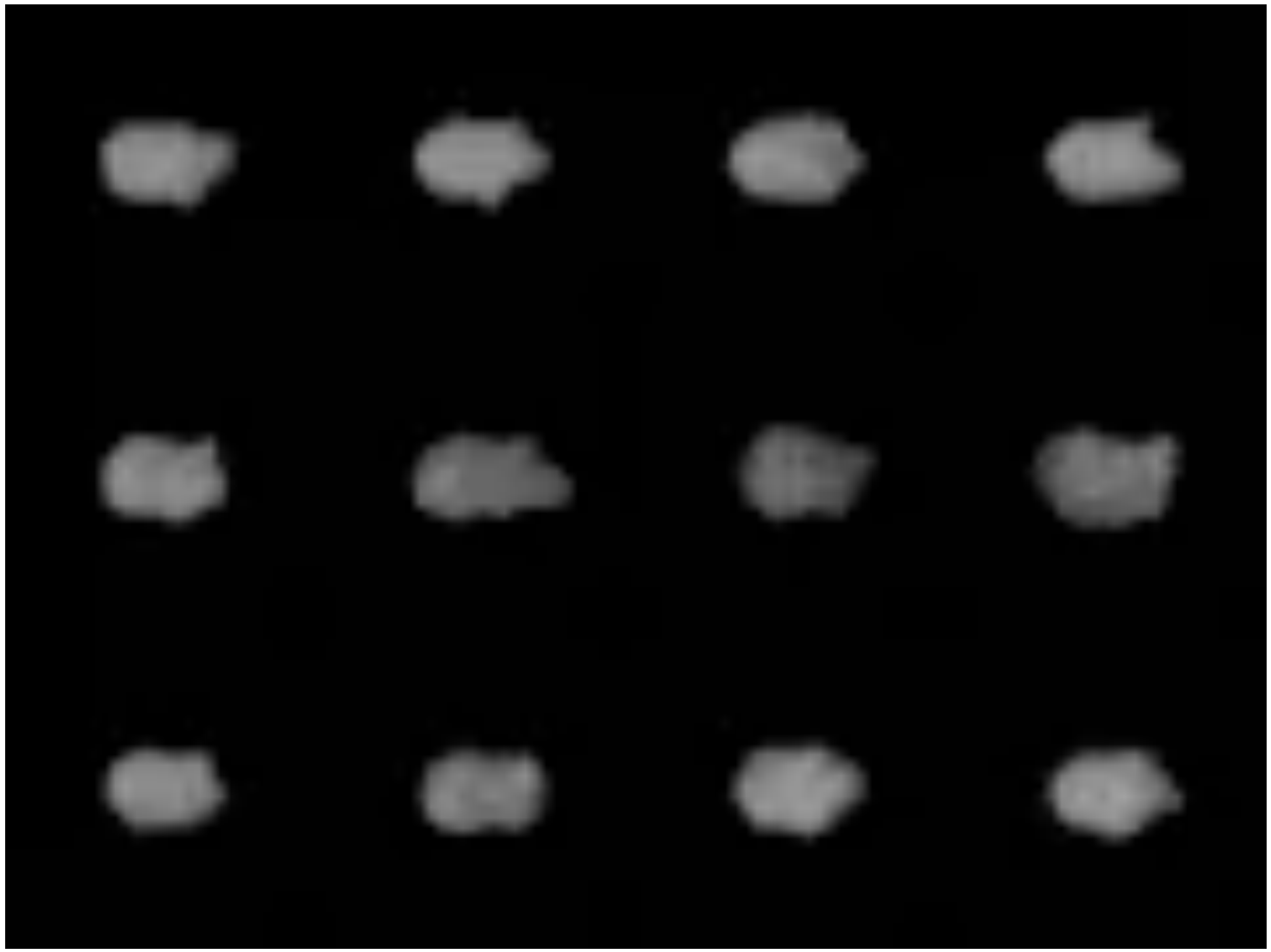
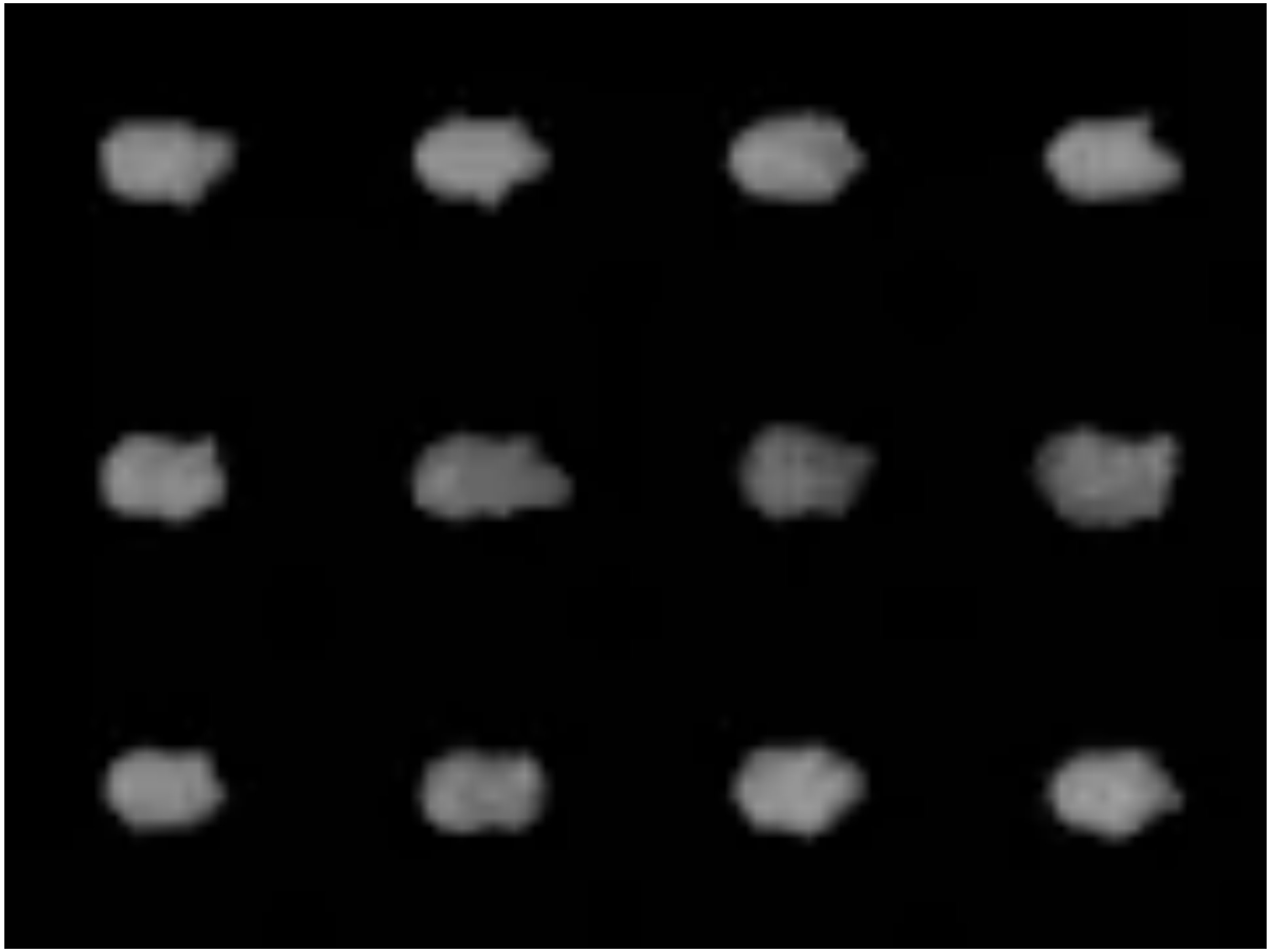
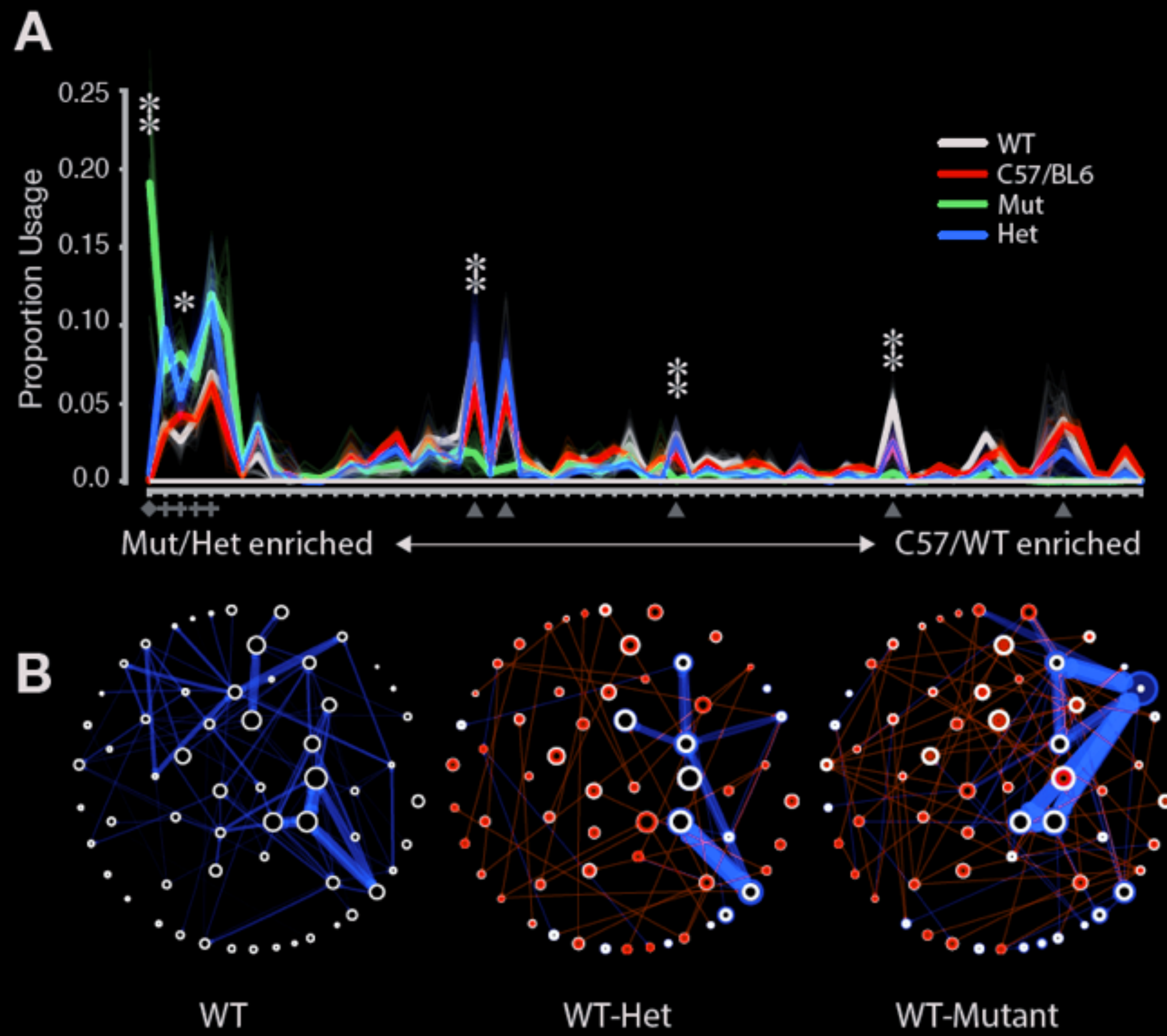


grooming



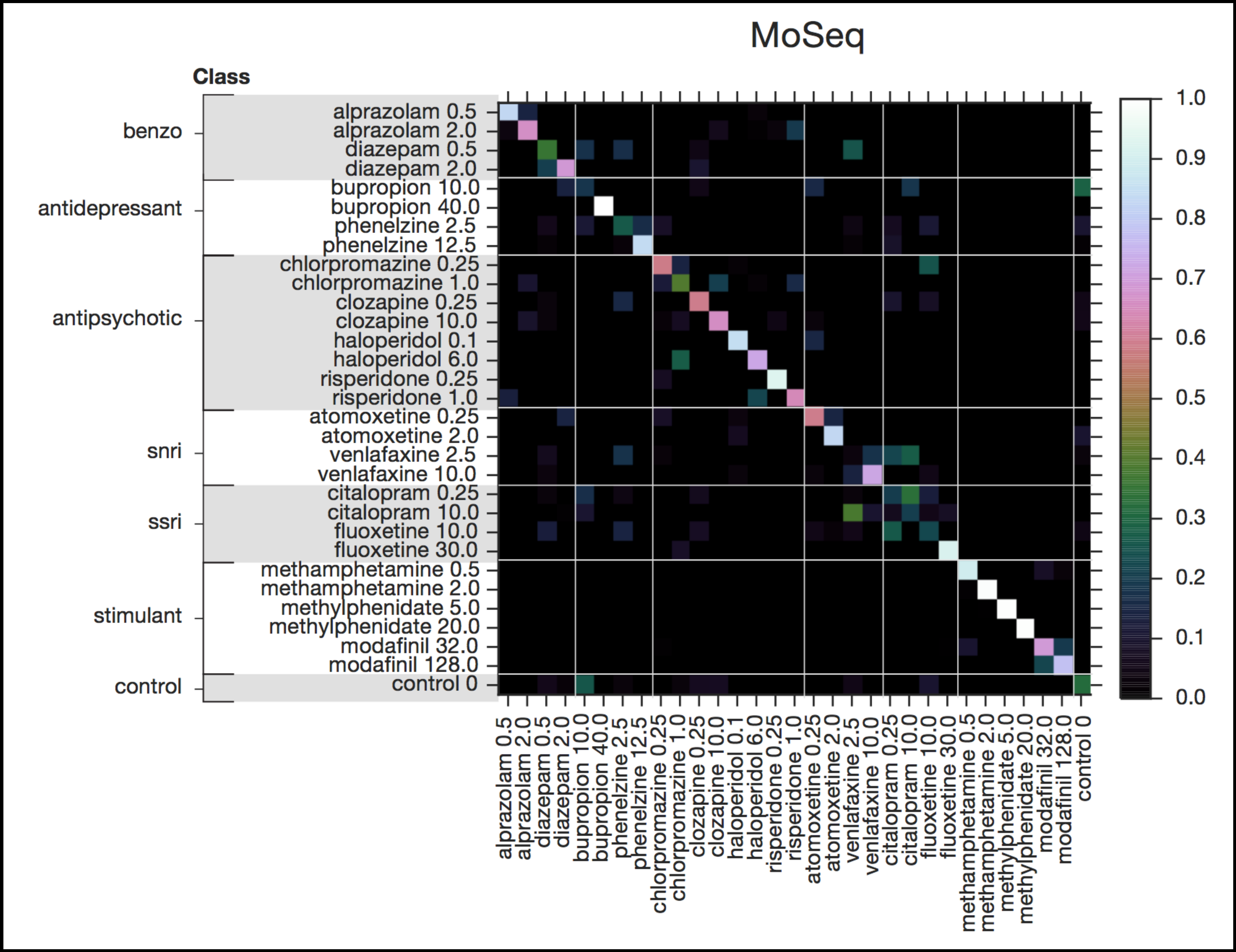
grooming

Discovery of Heterozygous Phenotypes in Ror1b Mice



Alexander Wiltschko, **Matthew Johnson**, et al., Neuron 2015.

… and high and low doses of each drug



from Alex Wiltschko preprint

Goals

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Non-goals

1. Cover the recent literature on PGMs + DNNs
2. Unpack all the technical details

What is JAX?

```
import jax.numpy as np
from jax import jit, grad, vmap

def predict(params, inputs):
  for W, b in params:
    outputs = np.dot(inputs, W) + b
    inputs = np.tanh(outputs)
  return outputs

def loss(params, batch):
  inputs, targets = batch
  preds = predict(params, inputs)
  return np.sum((preds - targets) ** 2)


gradient_fun = jit(grad(loss))
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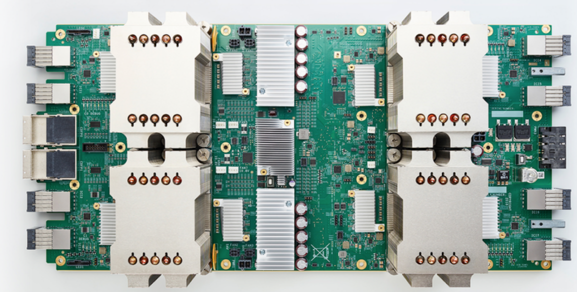

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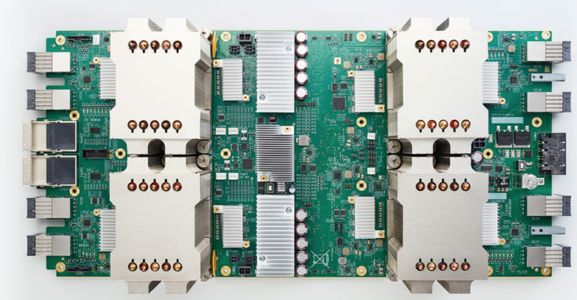

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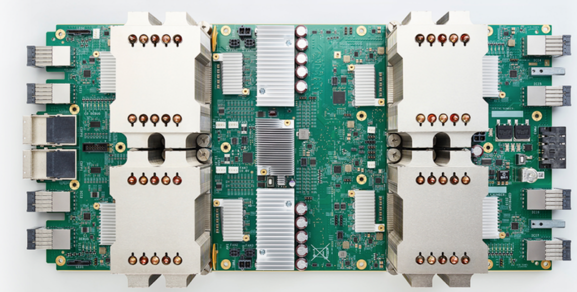

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JAX is an extensible system for
composable function transformations
of Python + NumPy code.

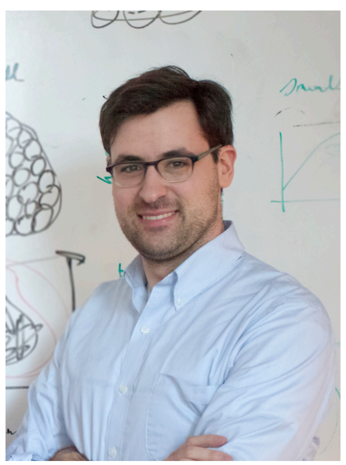
Composing graphical models with neural networks like chocolate and peanut butter

https://youtu.be/O7oD_oX-Gio

or

Graphical models and exponential families in the age of differentiable programming

David Duvenaud



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July 22 2019 @ UAI 2019