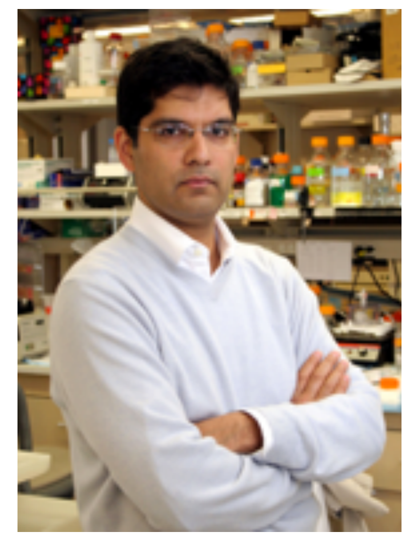
Composing graphical models with neural networks for structured representations and fast inference

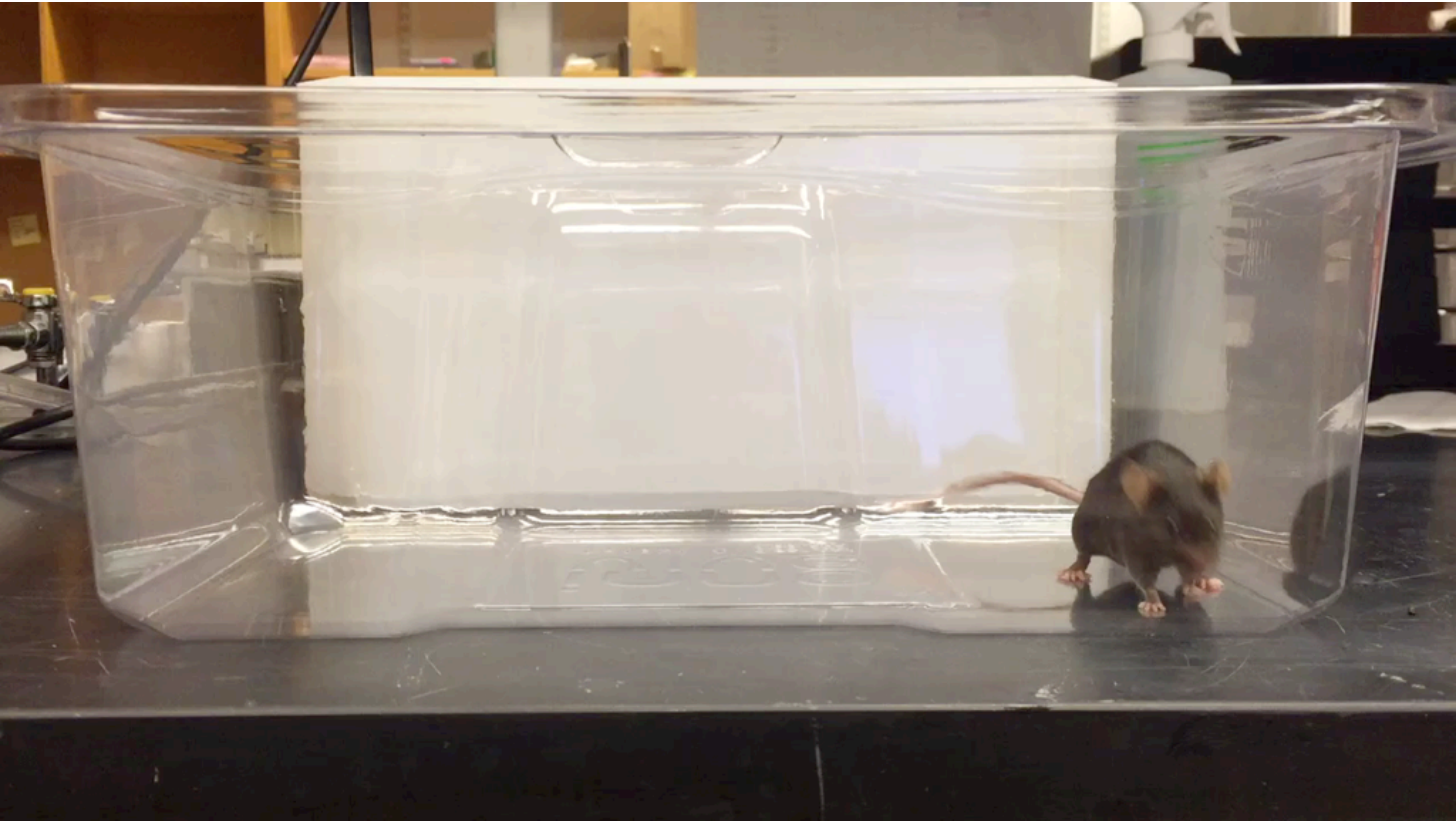
Matt Johnson, David Duvenaud, Alex Wiltschko, Bob Datta, Ryan Adams

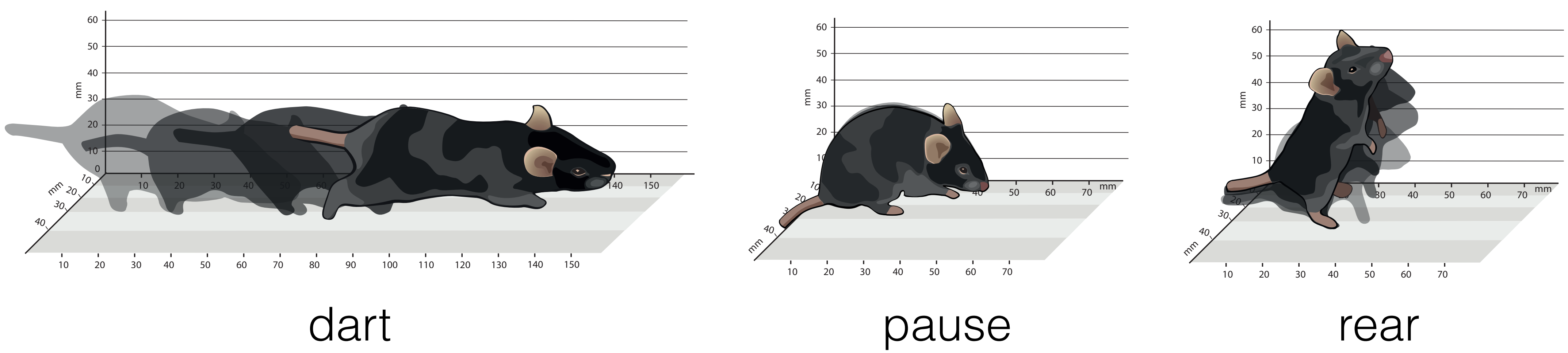


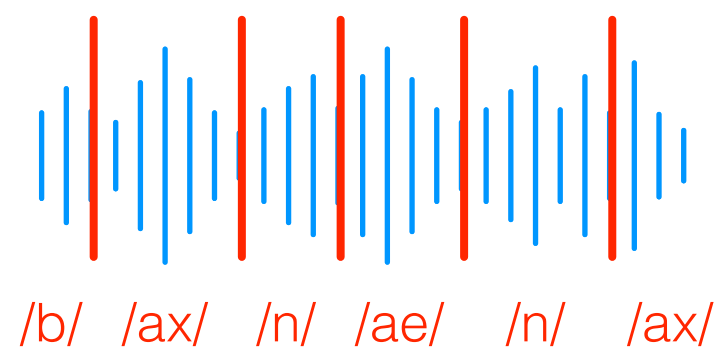




HARVARD INTELLIGENT PROBABILISTIC SYSTEMS

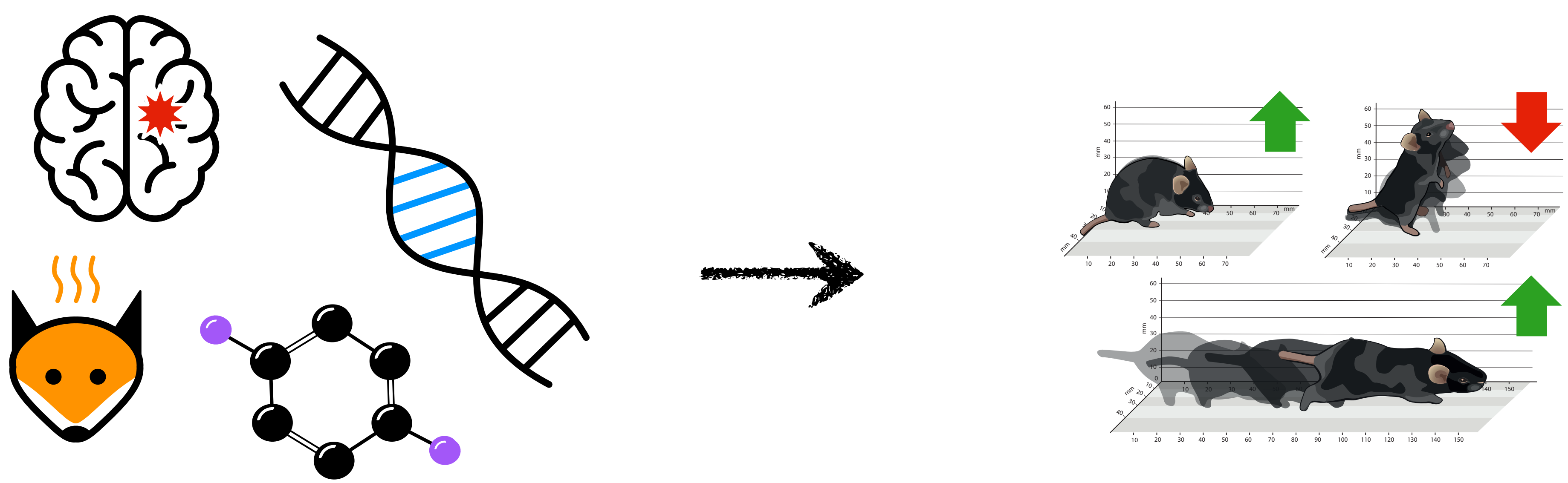
HARVARD MEDICAL SCHOOL



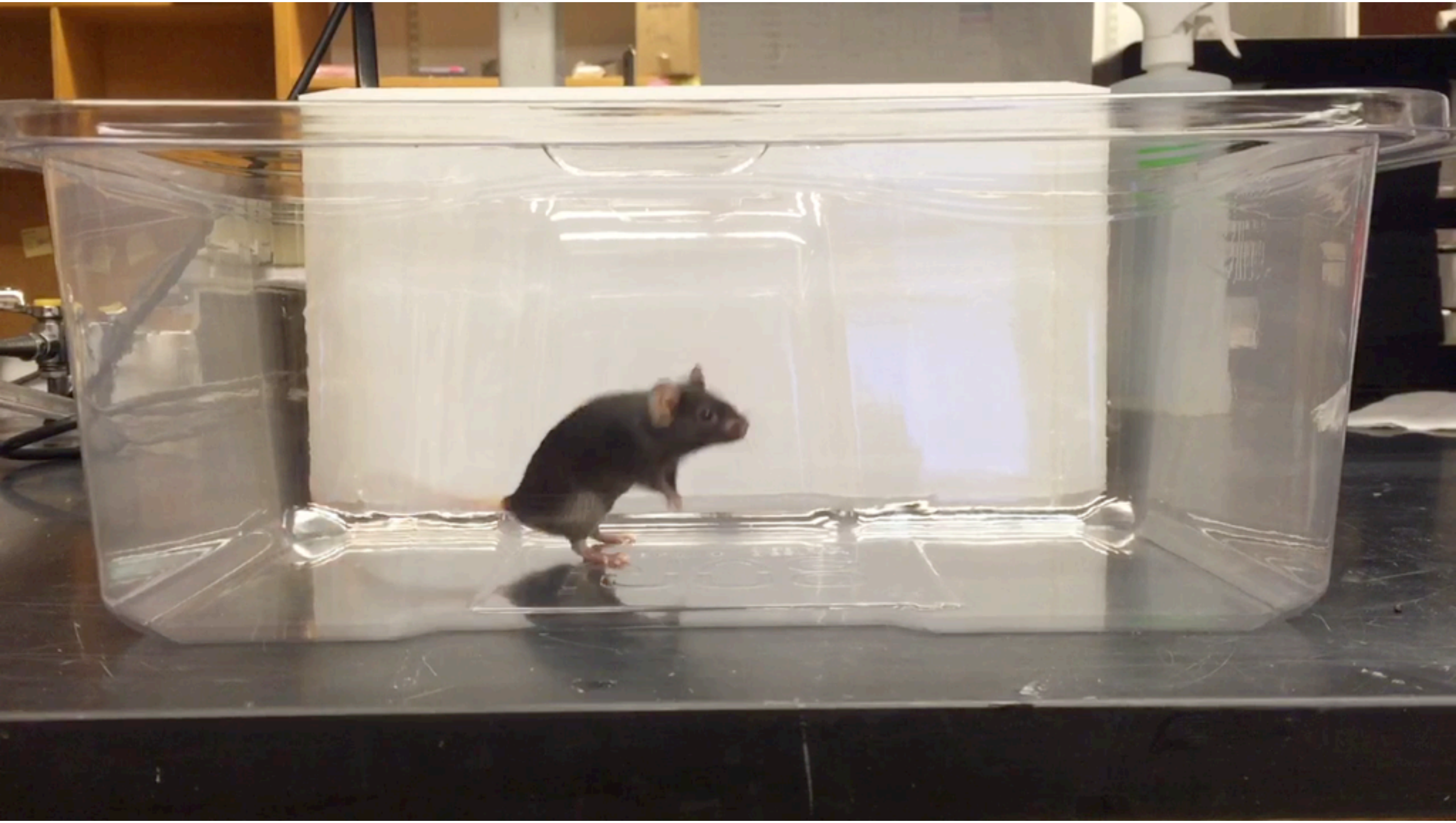


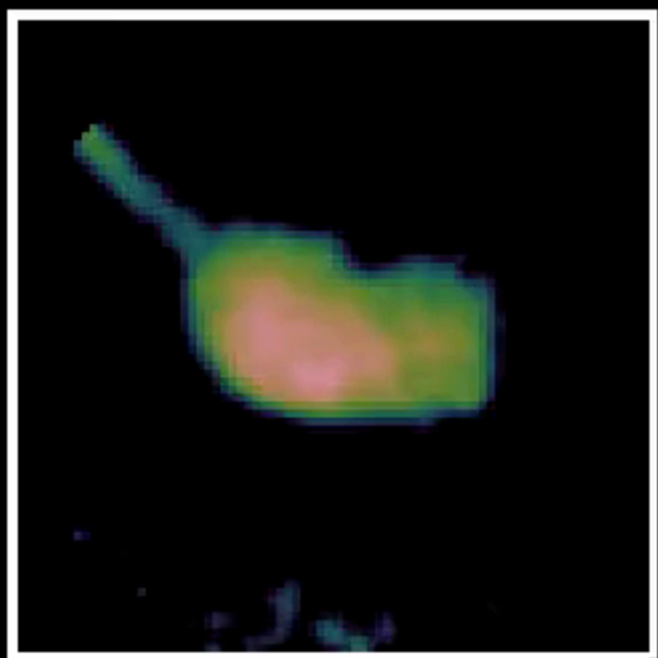


[1,2]



[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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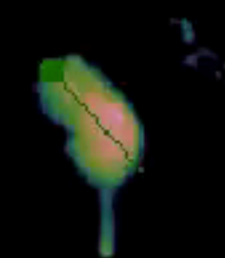
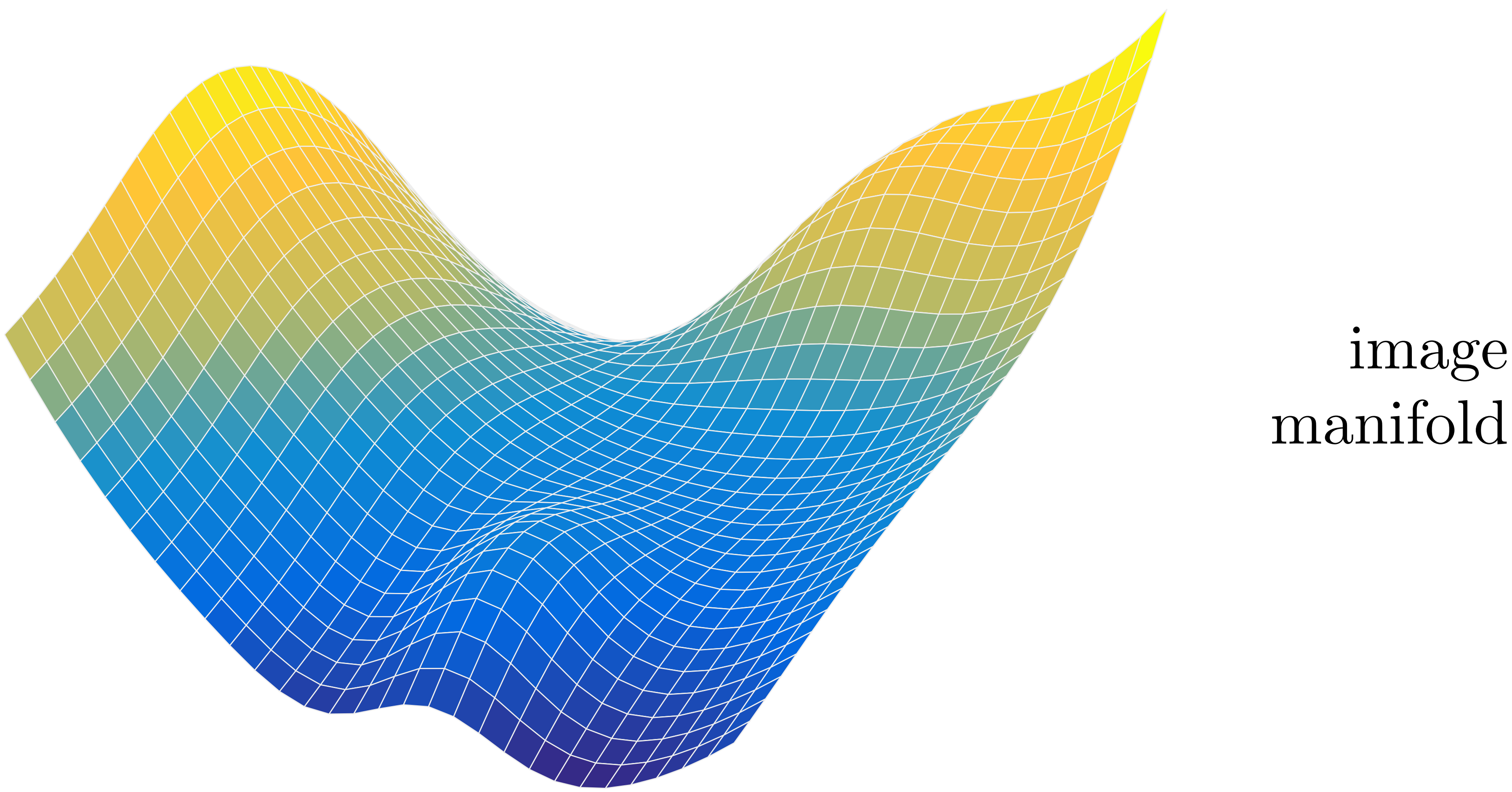


Alexander Wiltschko, **Matthew Johnson**, et al., Neuron 2015.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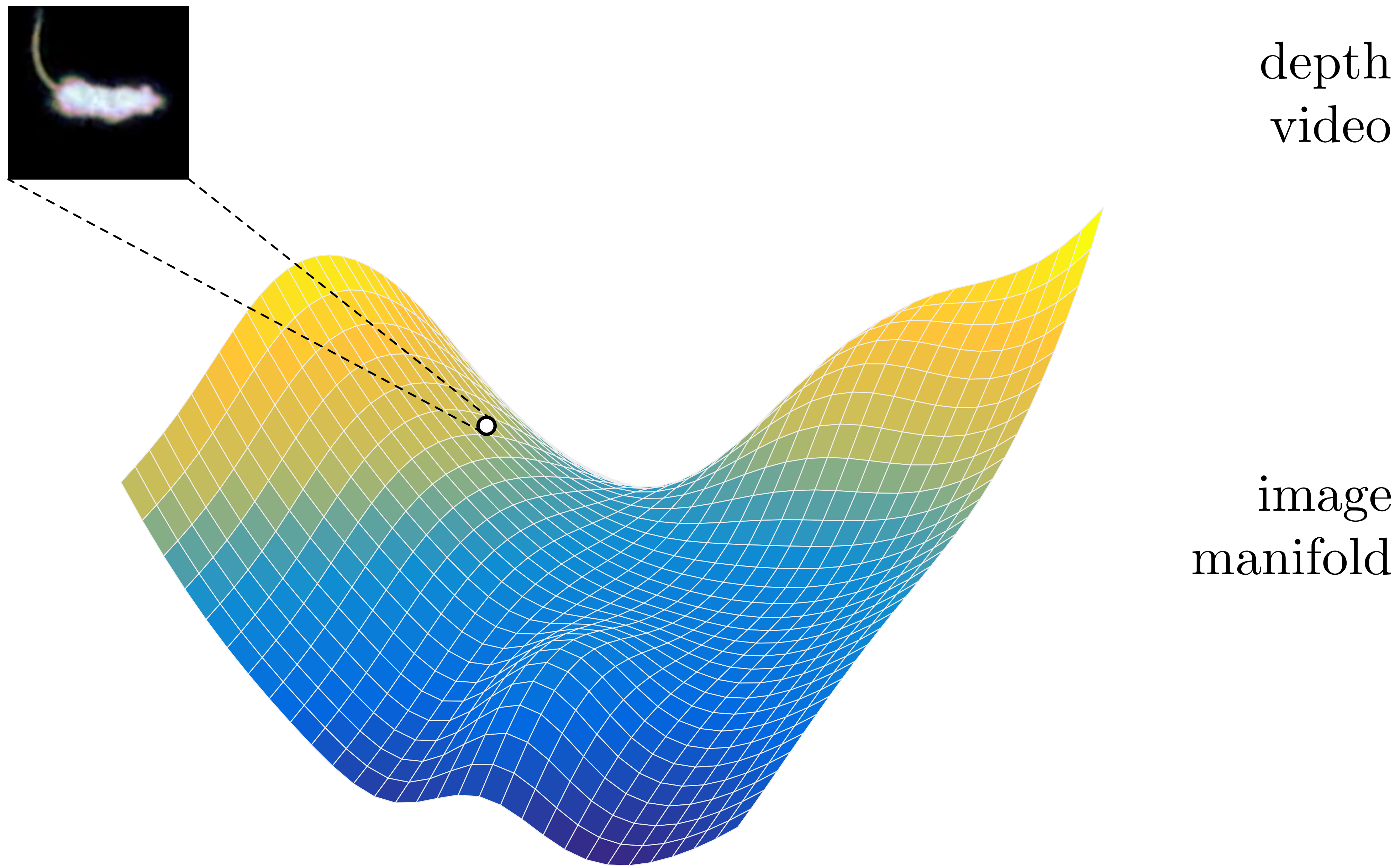
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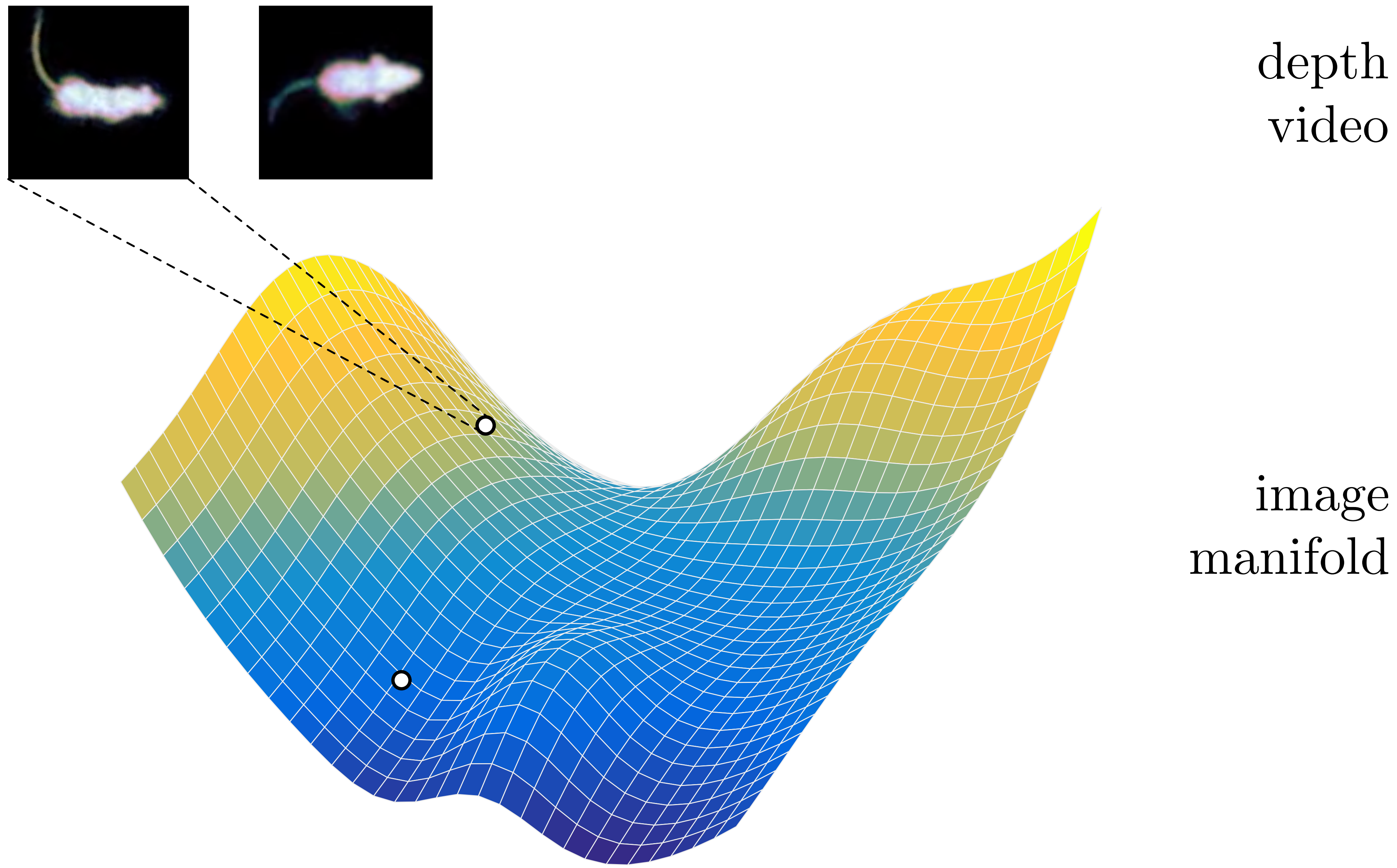
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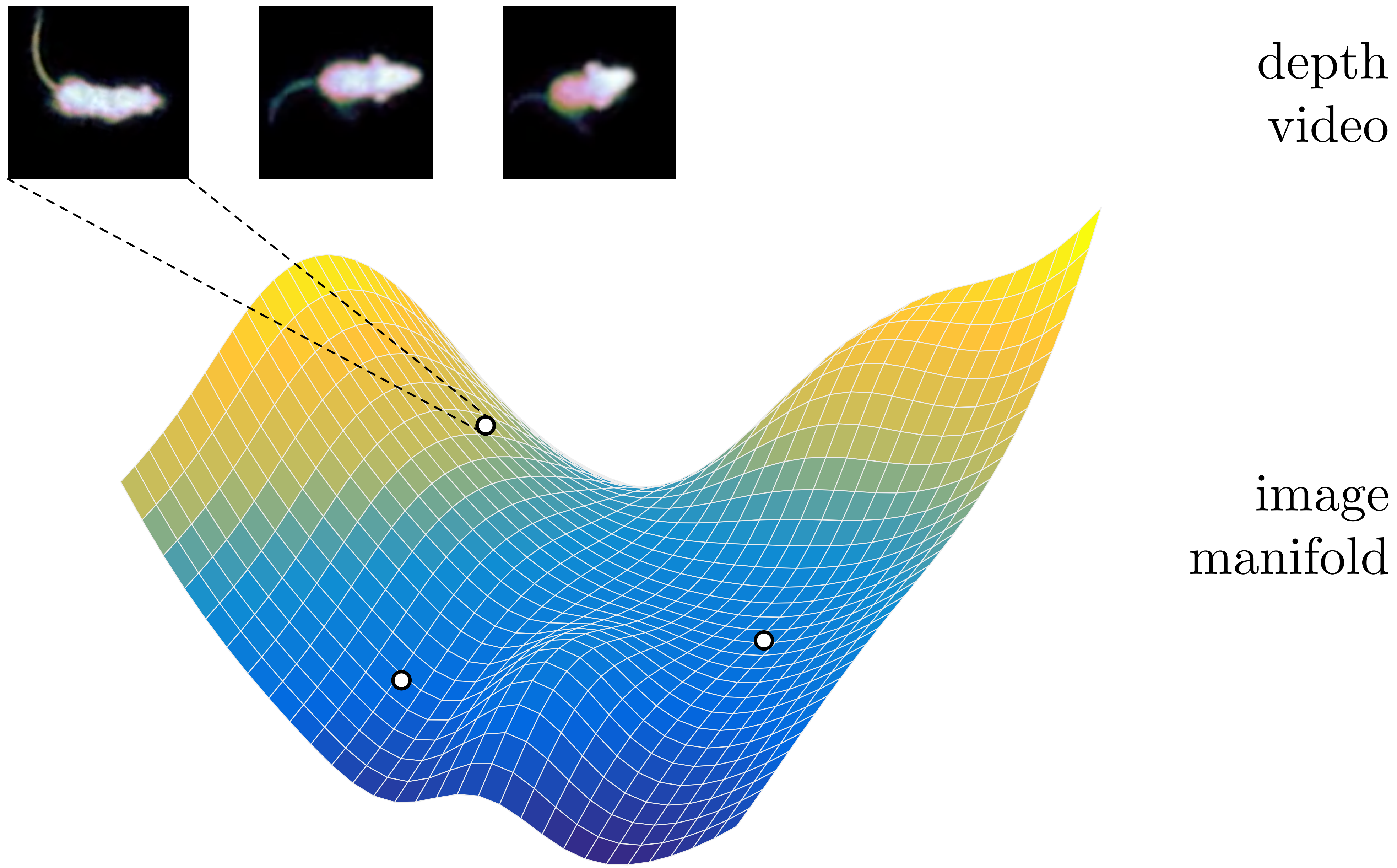
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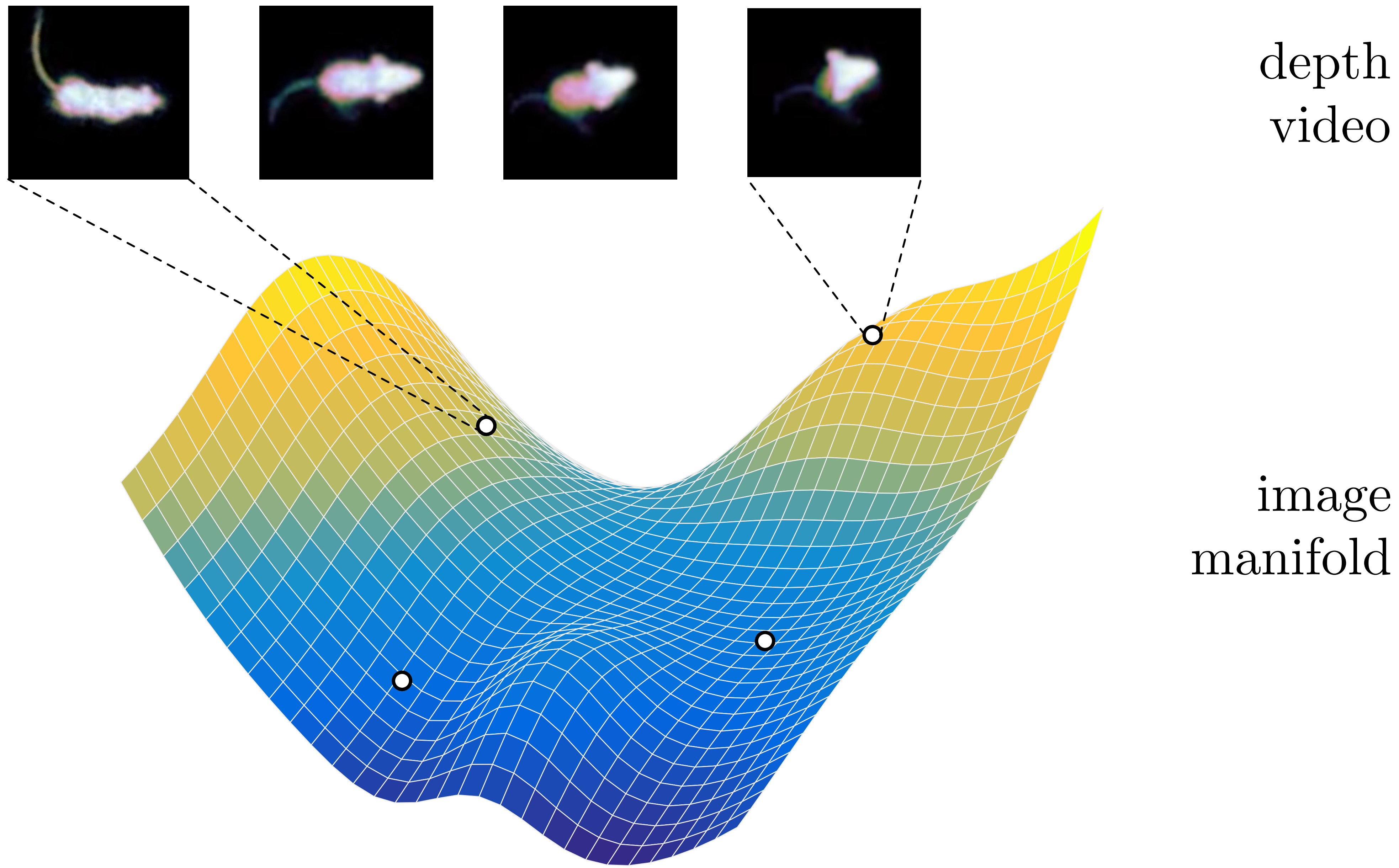
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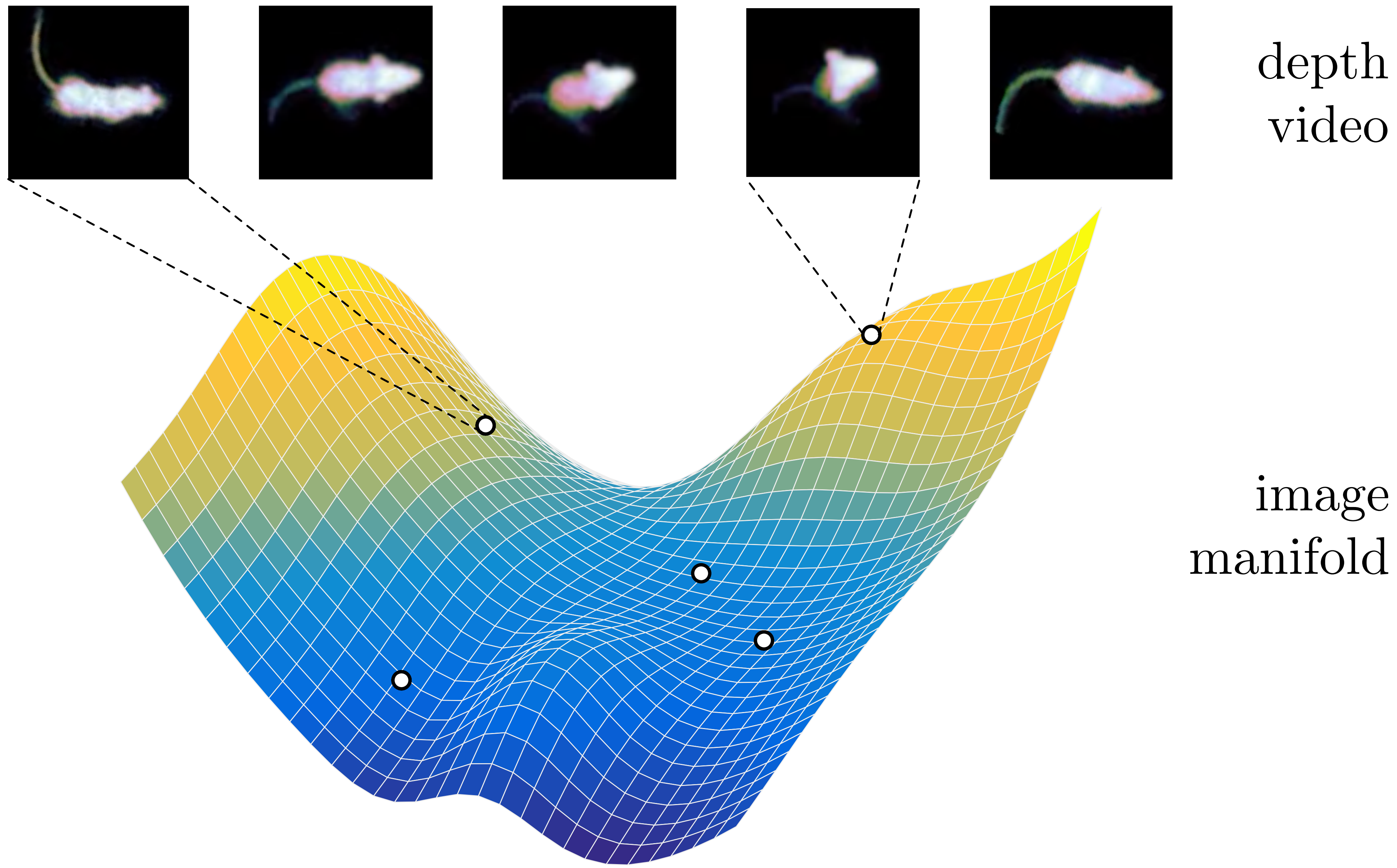
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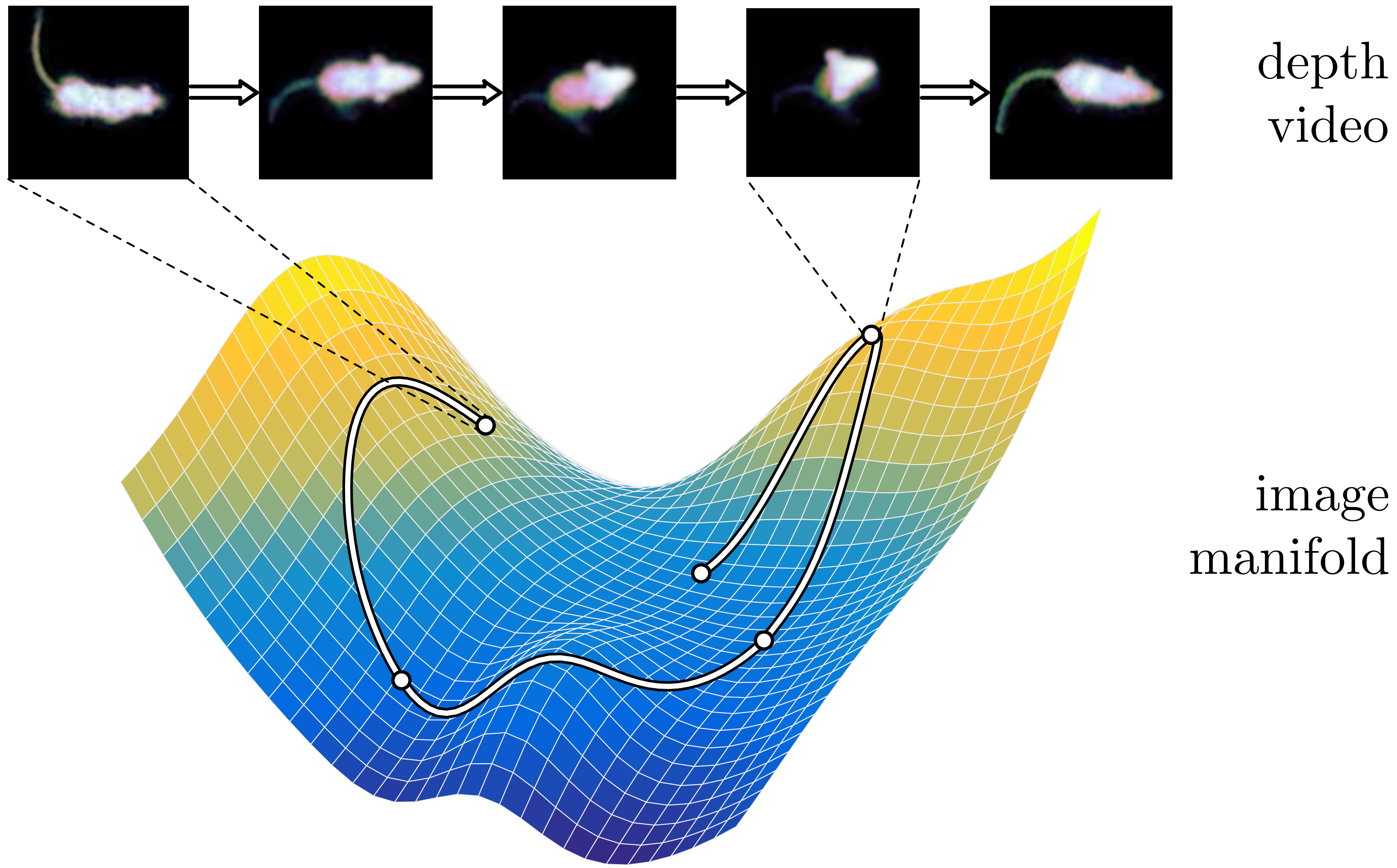
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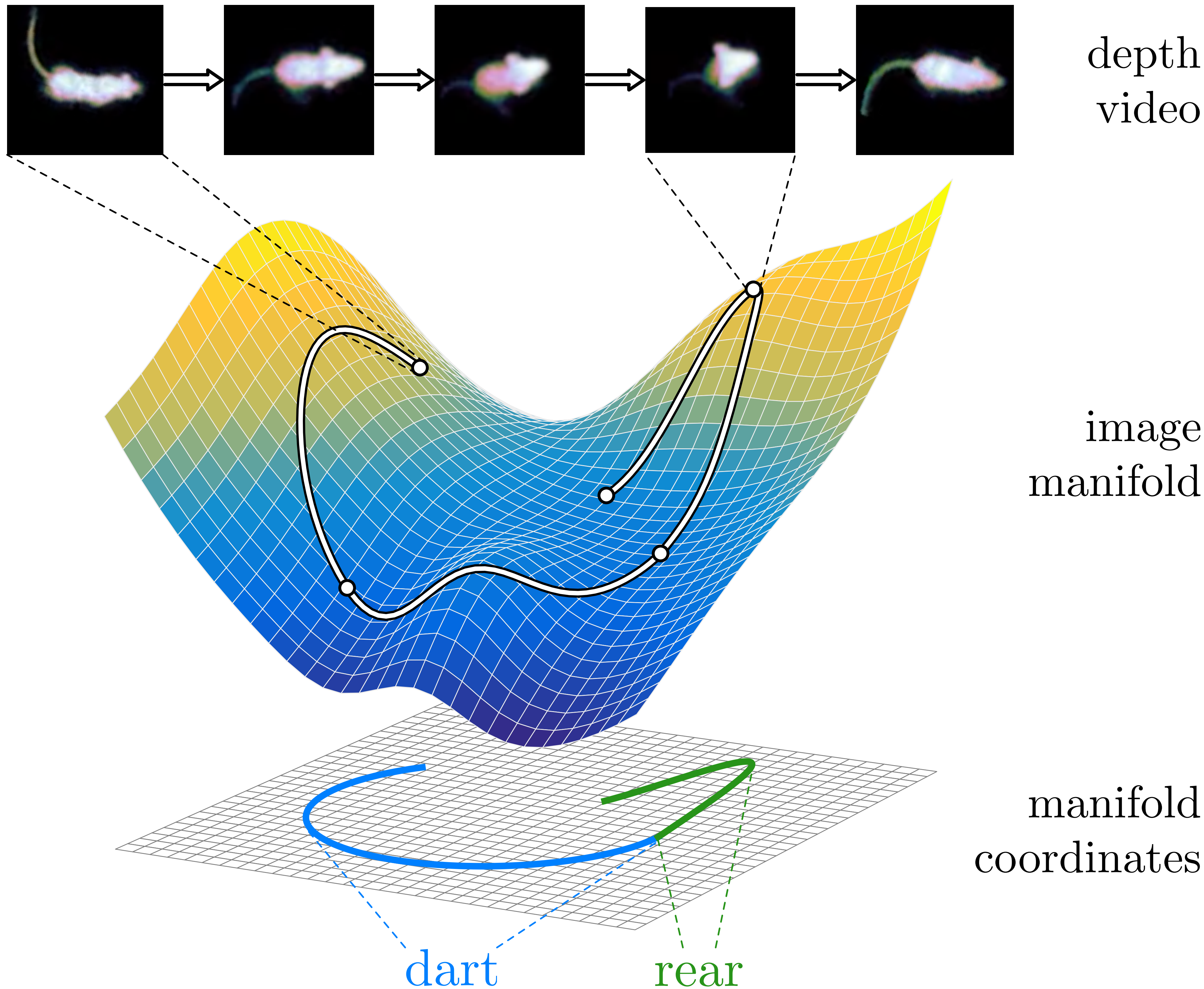
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Recurrent neural networks? [1,2,3]

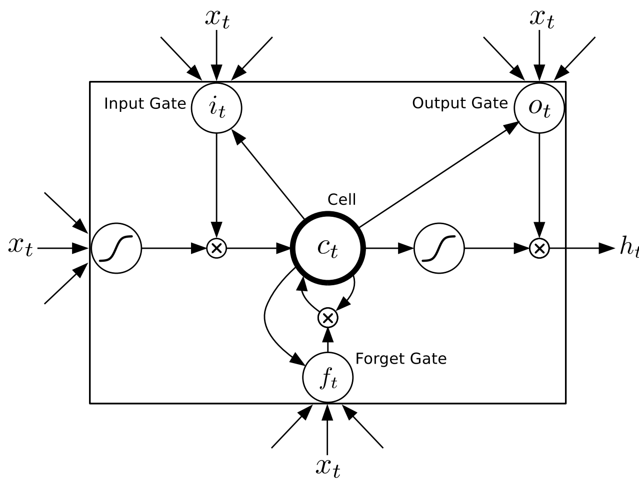


Figure 1. LSTM unit

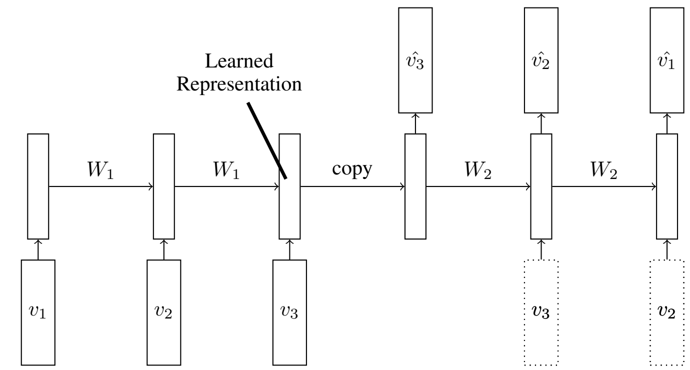
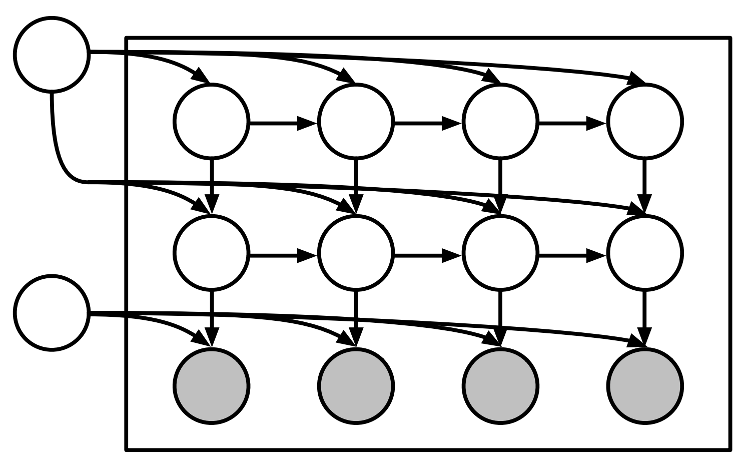
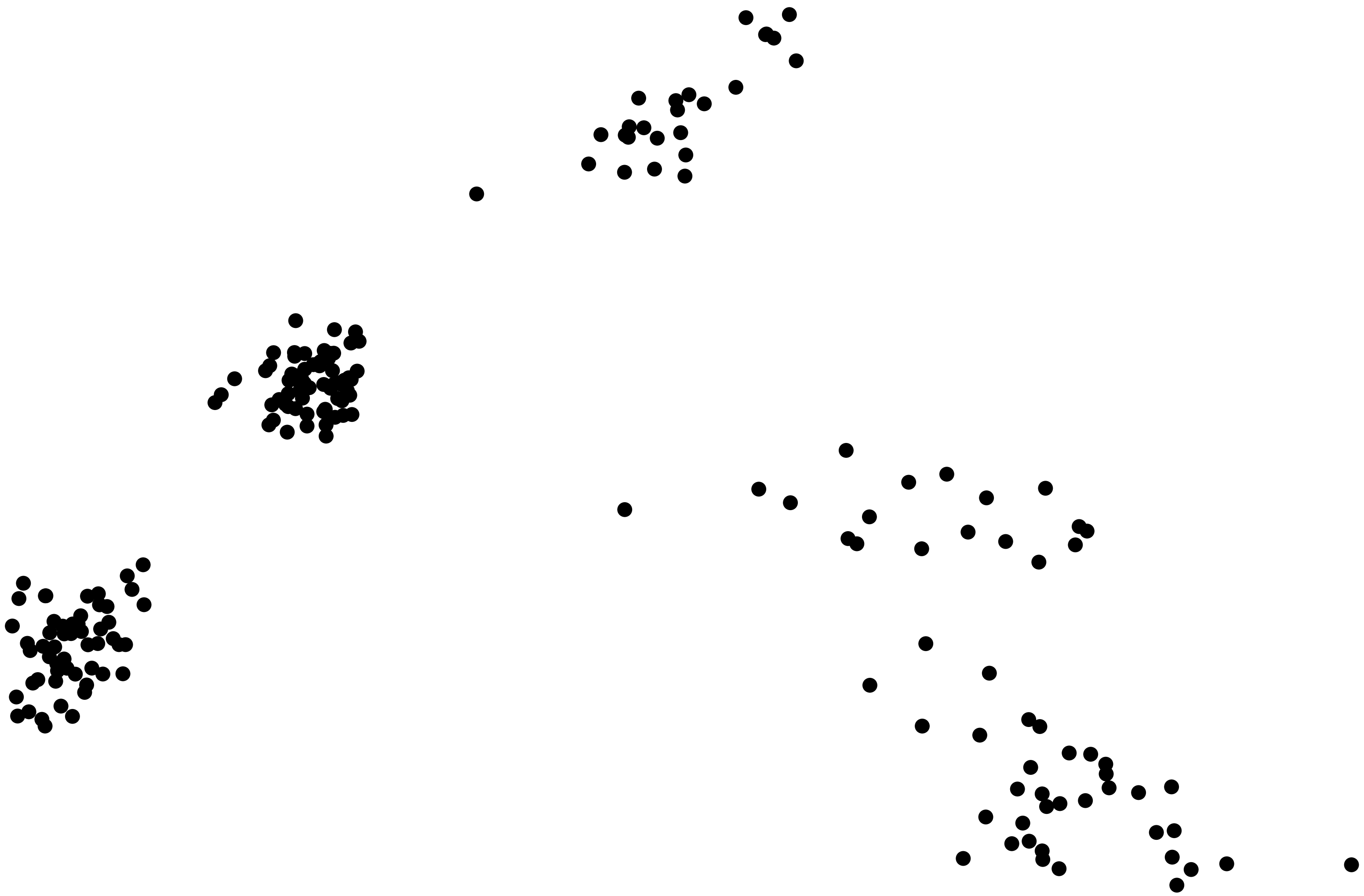


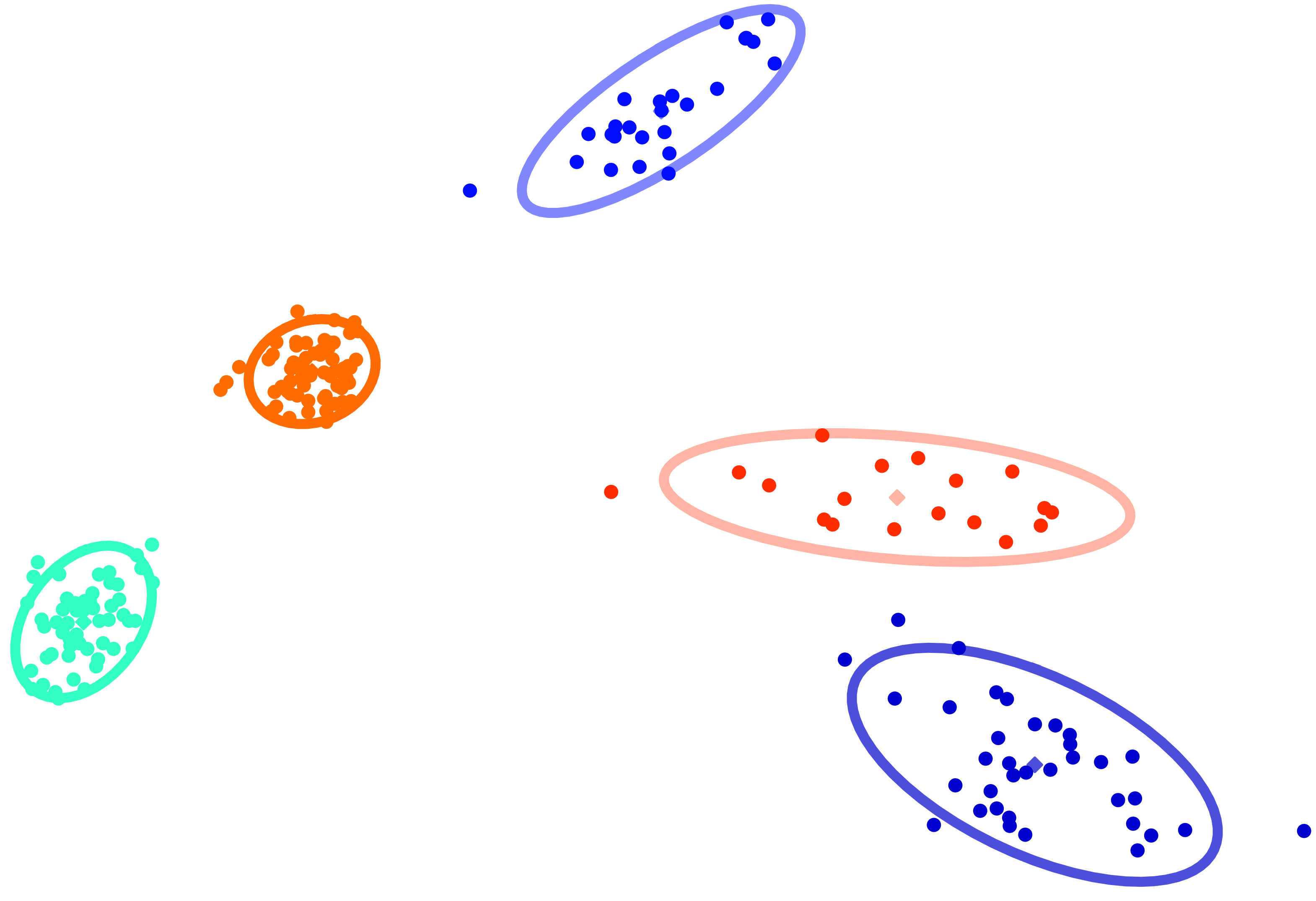
Figure 2. LSTM Autoencoder Model

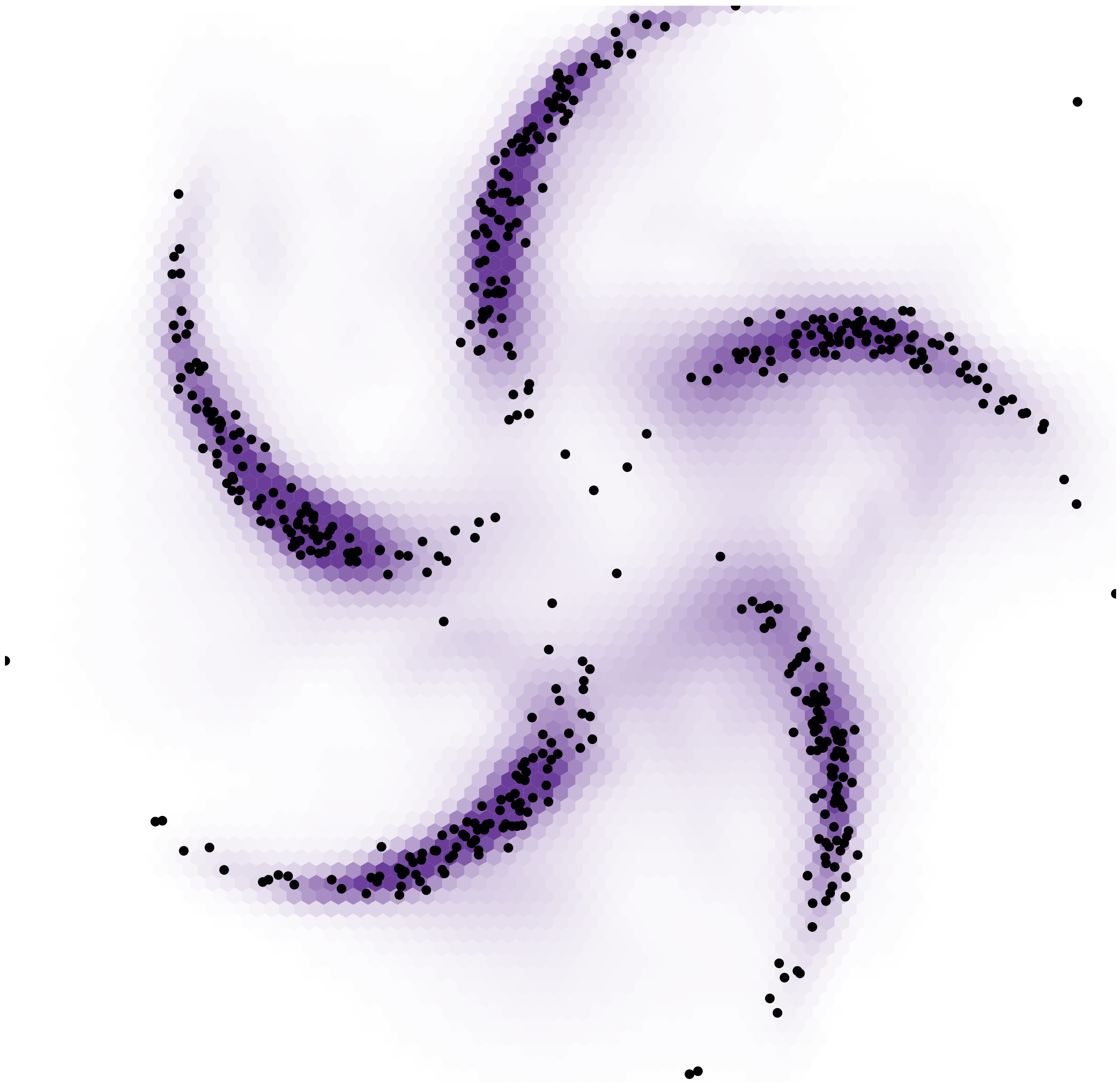
Probabilistic graphical models? [4,5,6]

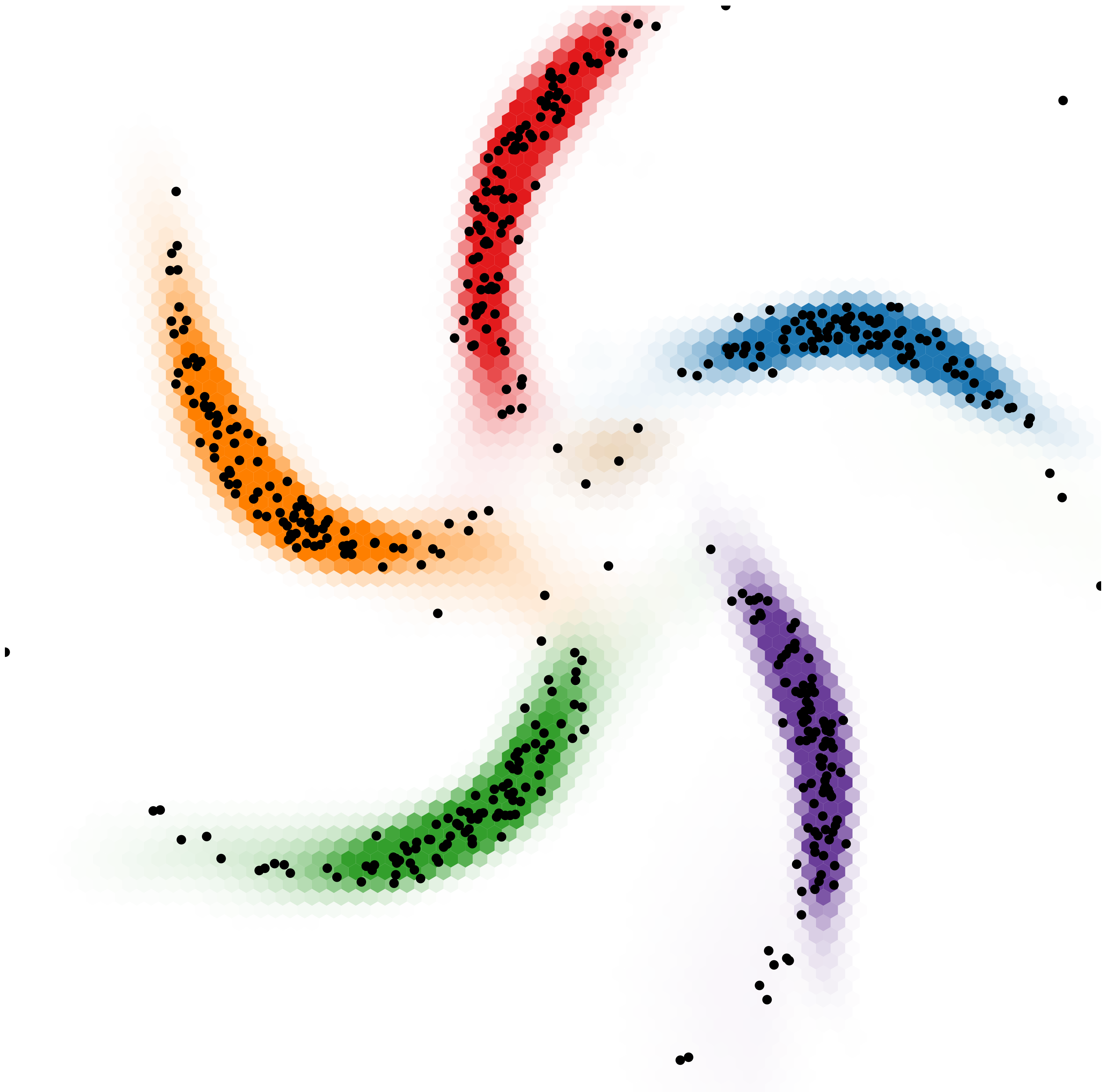


[1] Srivastava, Mansimov, Salakhutdinov. Unsupervised learning of video representations using LSTMs. ICML 2015.
[2] Ranzato, MarcAurelio, et al. Video (language) modeling: a baseline for generative models of natural videos. Preprint 2015.
[3] Sutskever, Hinton, and Taylor. The Recurrent Temporal Restricted Boltzmann Machine. NIPS 2008.
[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.

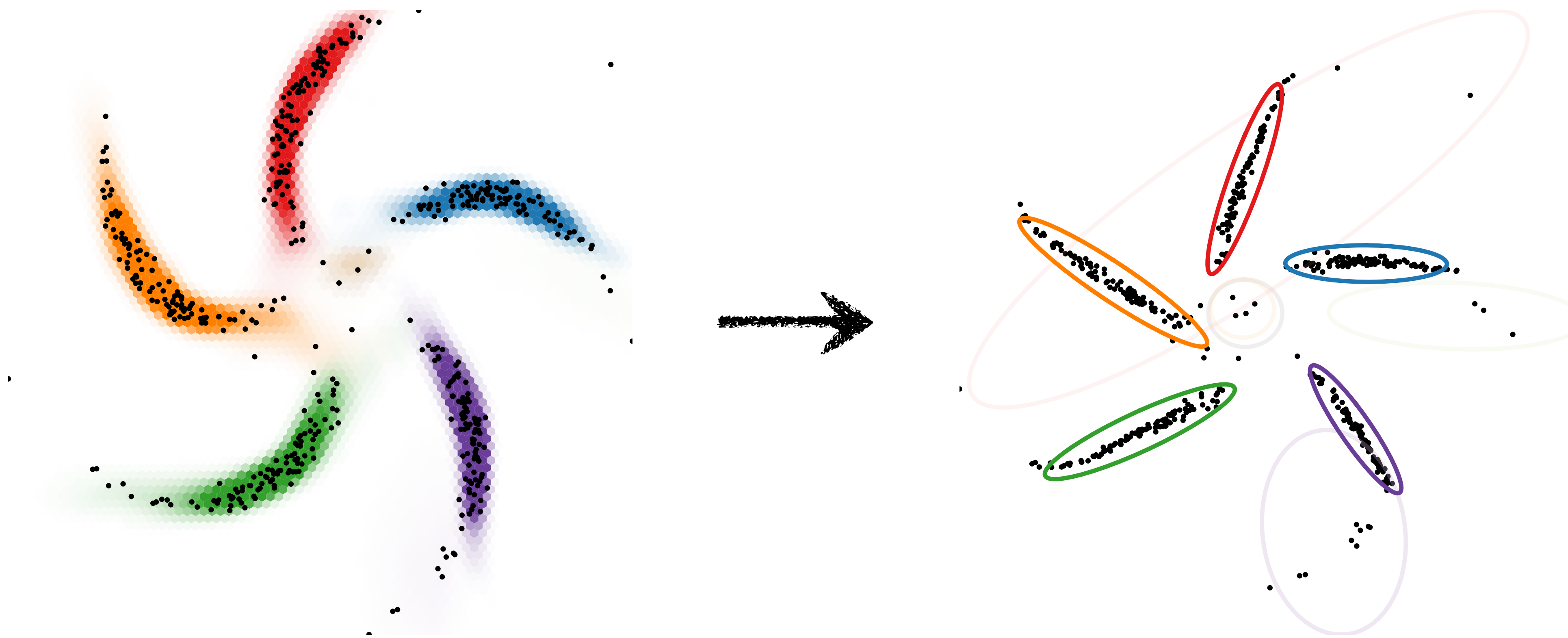




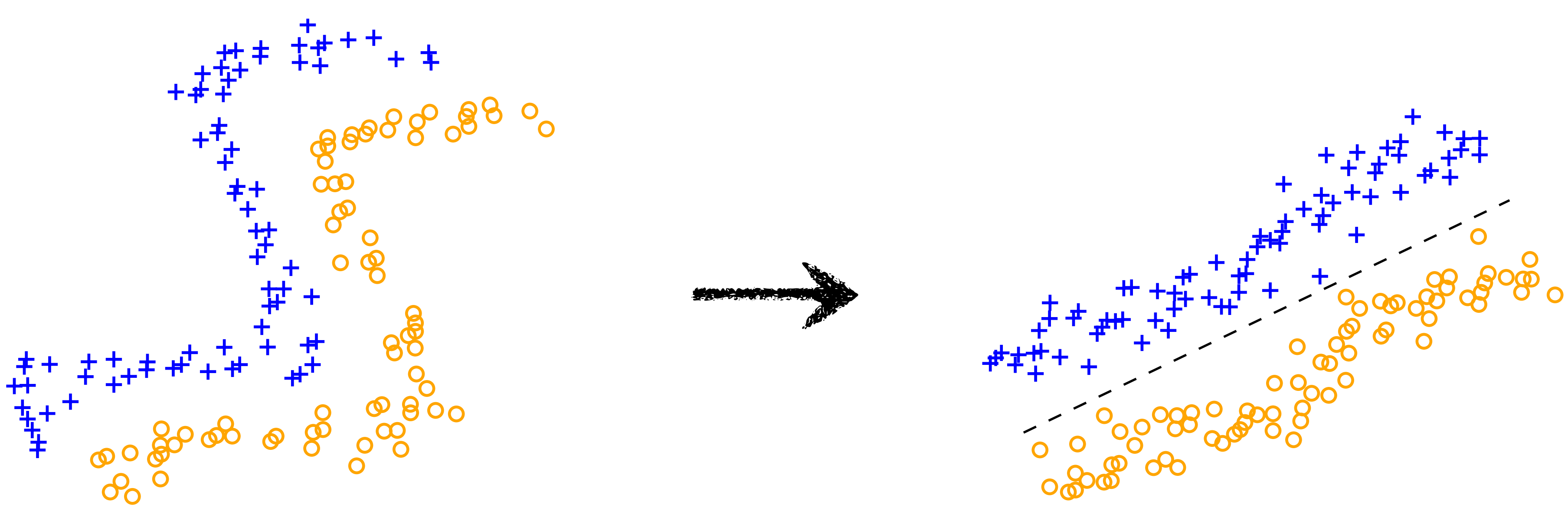




unsupervised learning



supervised learning



Probabilistic graphical models

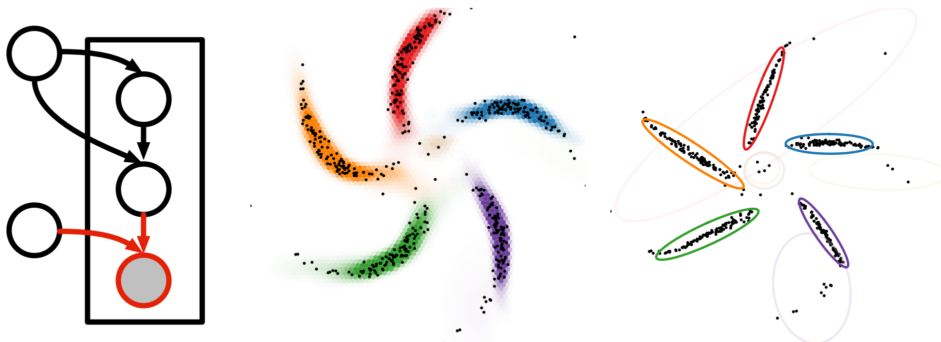
+ structured representations
+ priors and uncertainty
+ data and computational efficiency
– rigid assumptions may not fit
– feature engineering
– top-down inference

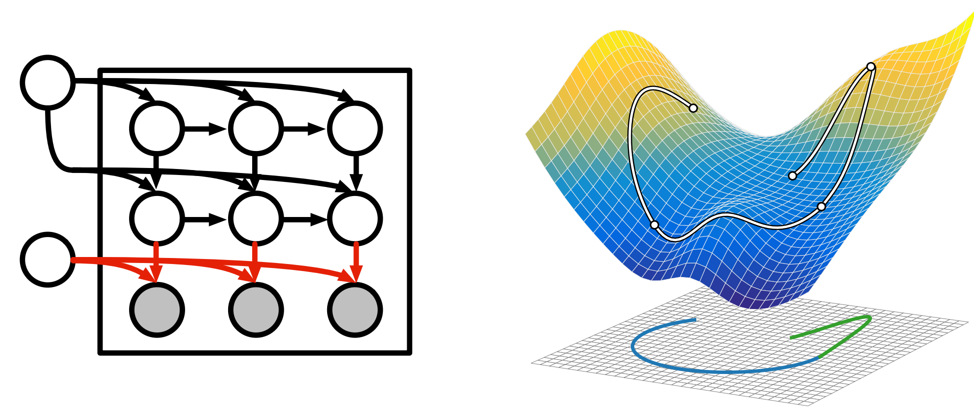
Deep learning

– neural net “goo”
– difficult parameterization
– can require lots of data
+ flexible
+ feature learning
+ recognition networks

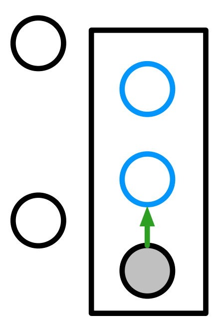

MAKE PGMS
GREAT AGAIN

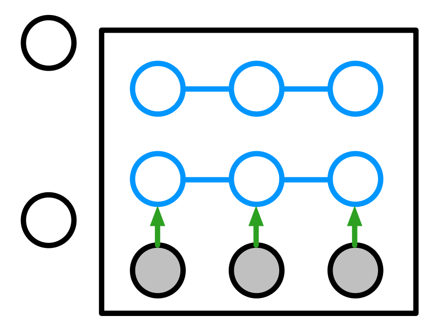
Modeling idea: graphical models on latent variables, neural network models for observations



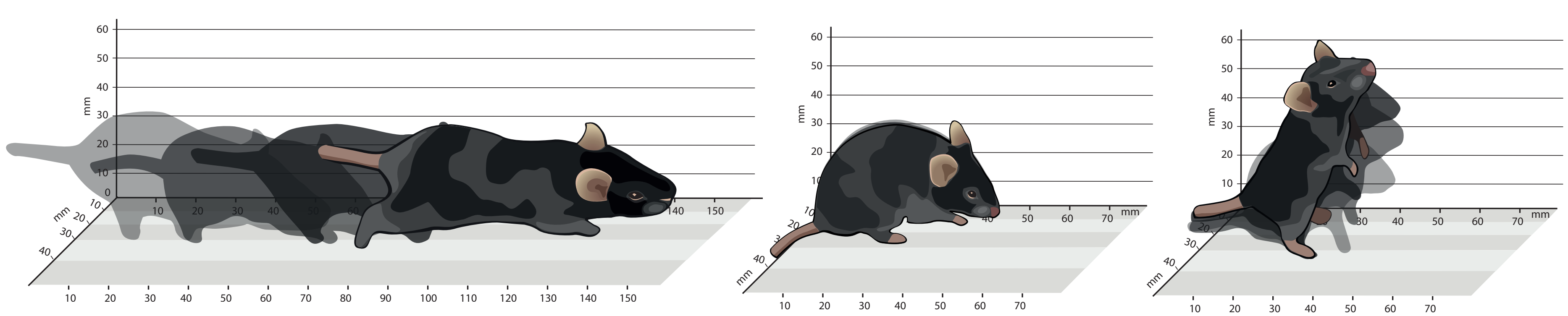


Inference: recognition networks output conjugate potentials, then apply fast graphical model inference

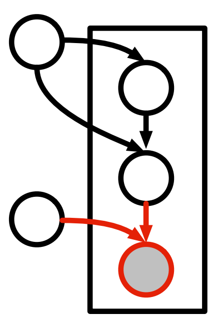


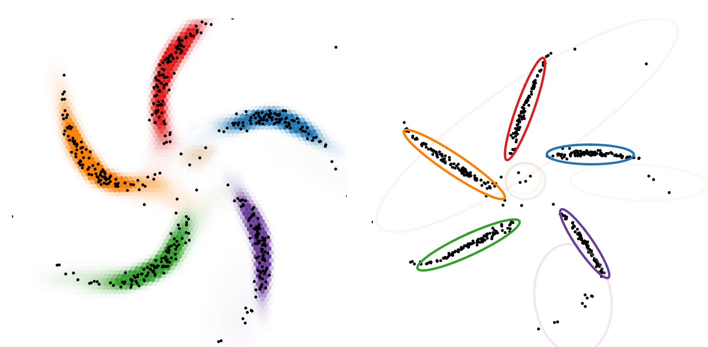


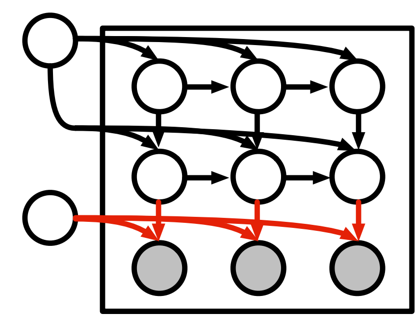
Application: learn syllable representation of behavior from video

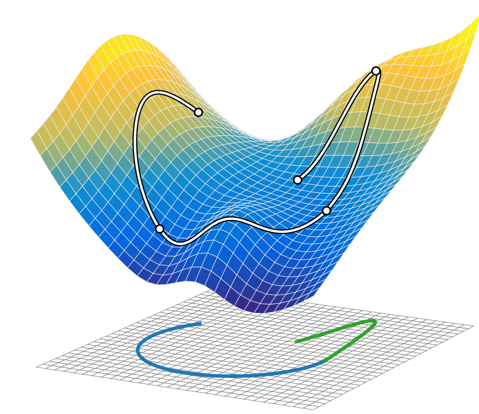


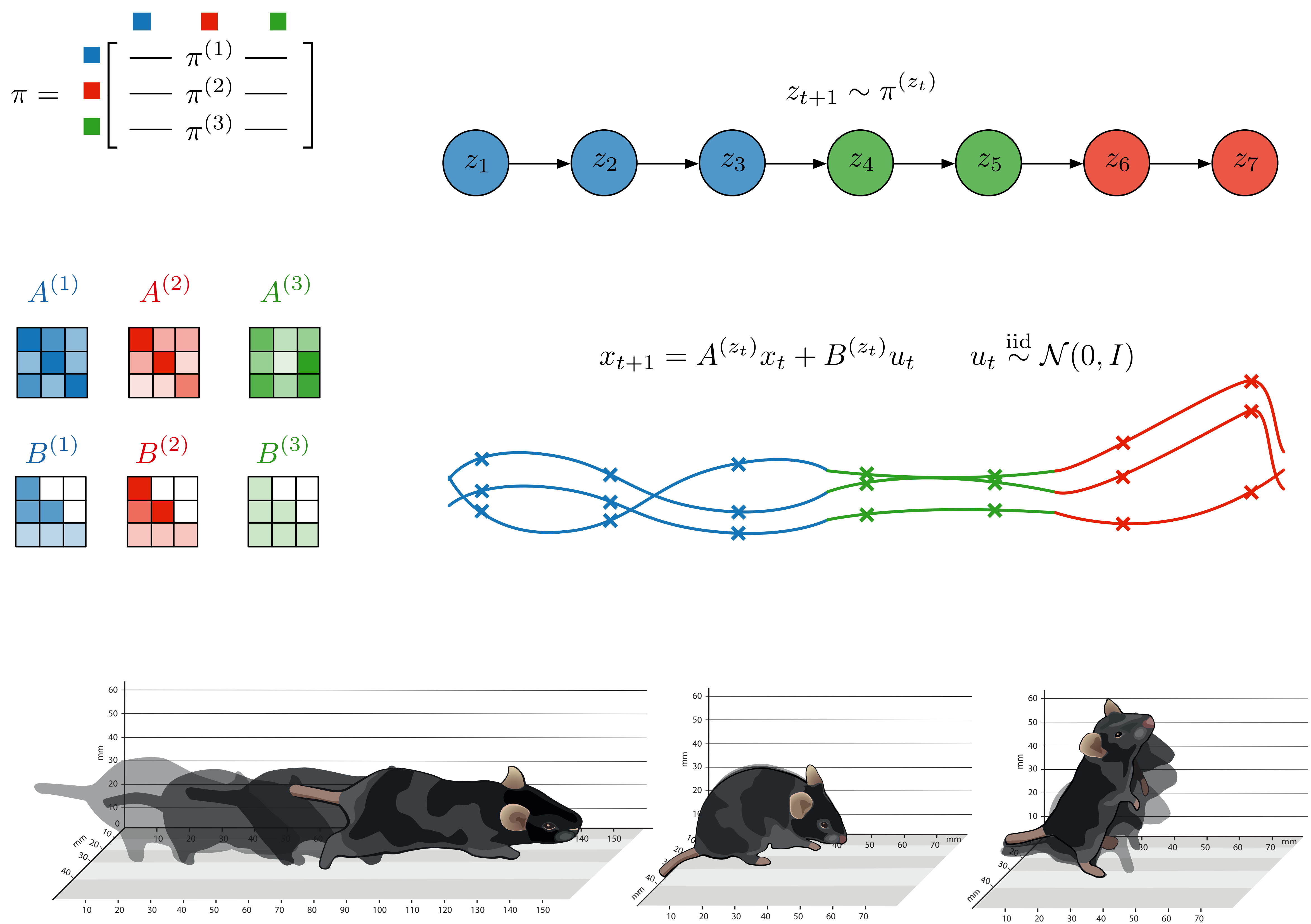
Modeling idea: graphical models on latent variables,
neural network models for observations



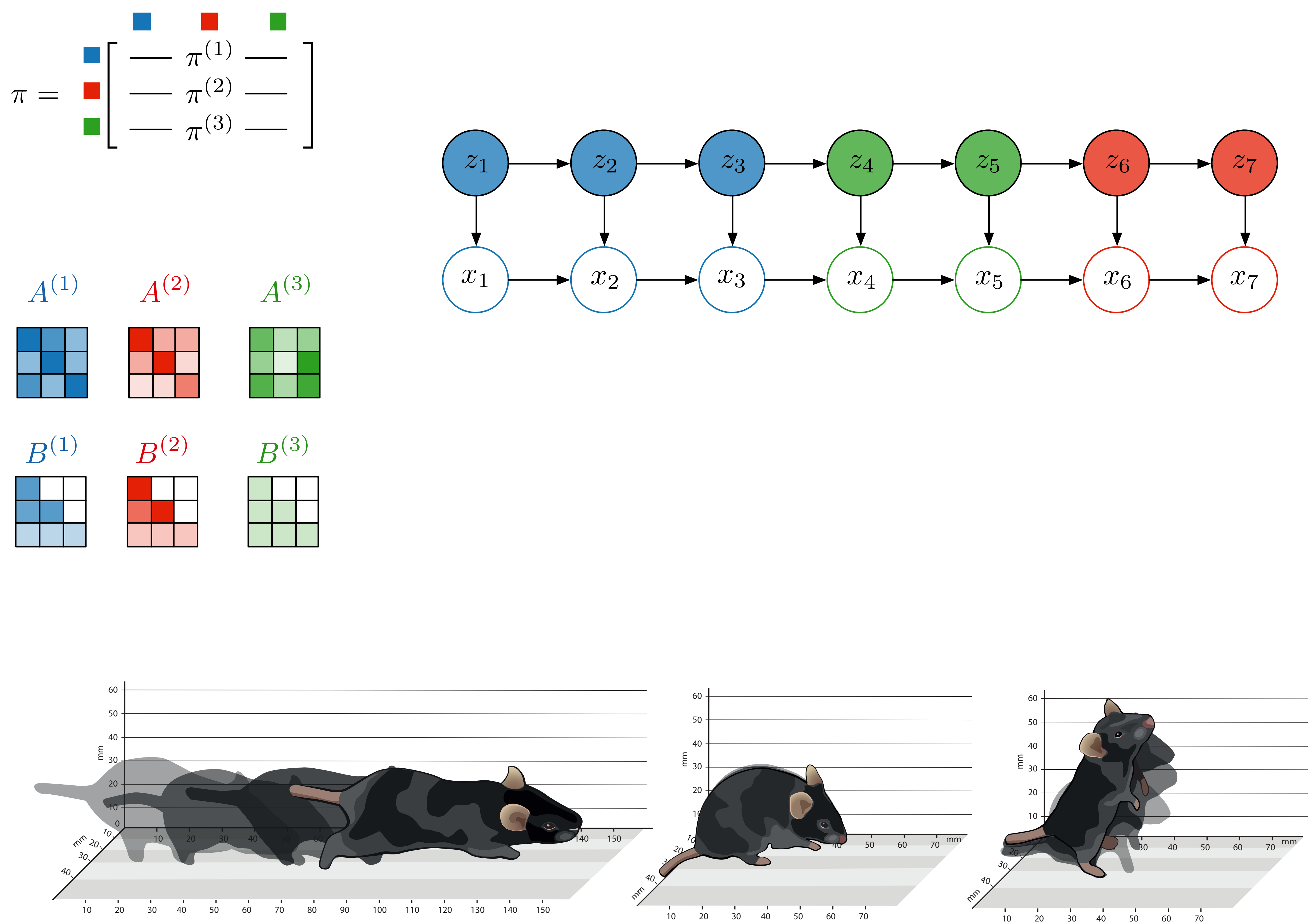




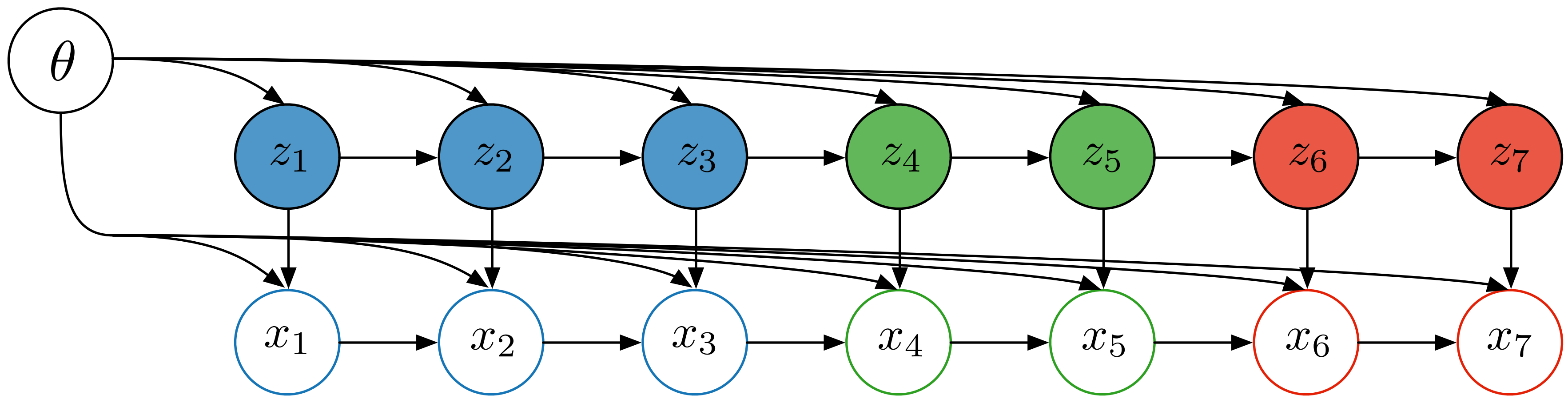




$\pi = \begin{bmatrix} — \pi^{(1)} — \\ — \pi^{(2)} — \\ — \pi^{(3)} — \end{bmatrix}$
$z_{t+1} \sim \pi^{(z_t)}$
z_1 z_2 z_3 z_4 z_5 z_6 z_7
$A^{(1)}$ $A^{(2)}$ $A^{(3)}$
$B^{(1)}$ $B^{(2)}$ $B^{(3)}$
$x_{t+1} = A^{(z_t)} x_t + B^{(z_t)} u_t \qquad u_t \overset{\text{iid}}{\sim} \mathcal{N}(0, I)$
mm



$\pi =$
$\pi^{(1)}$
$\pi^{(2)}$
$\pi^{(3)}$
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
$A^{(1)}$ $A^{(2)}$ $A^{(3)}$
$B^{(1)}$ $B^{(2)}$ $B^{(3)}$
mm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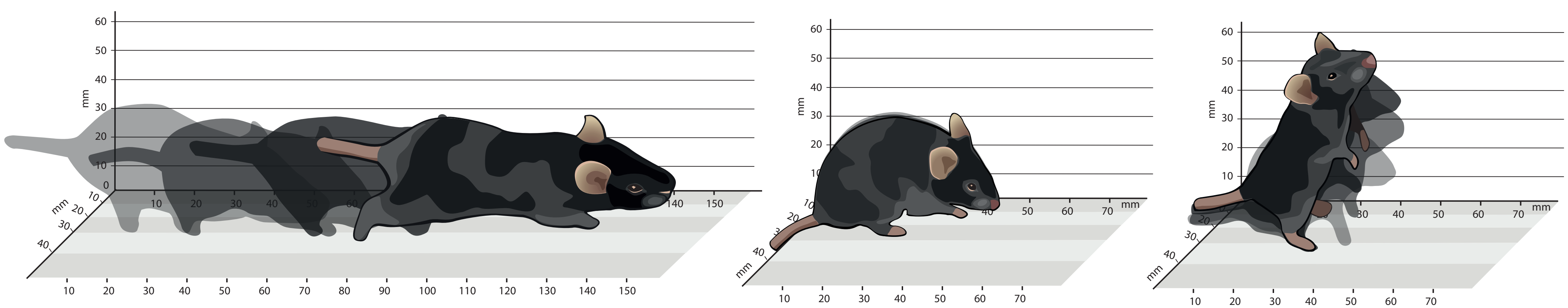
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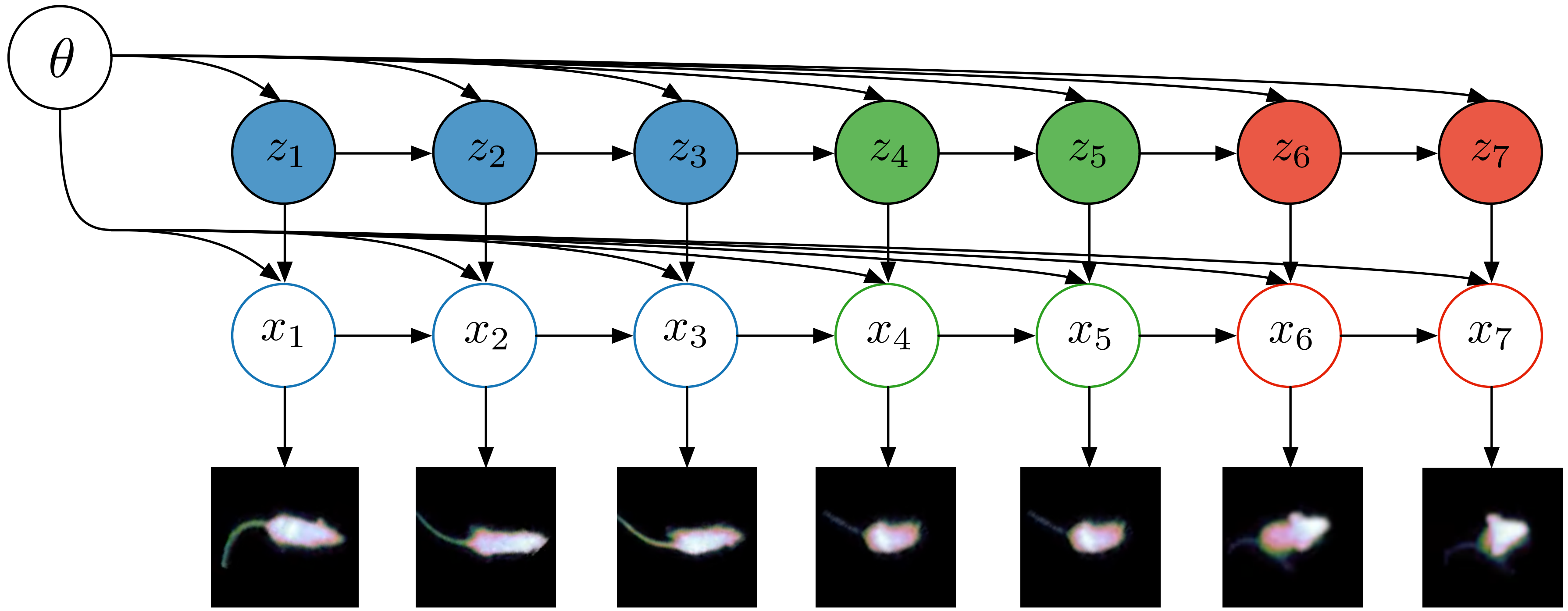

θ
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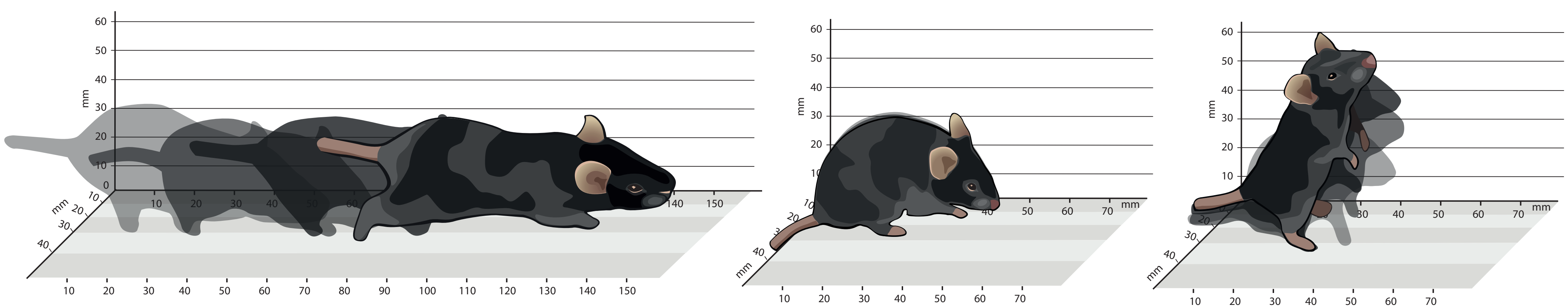

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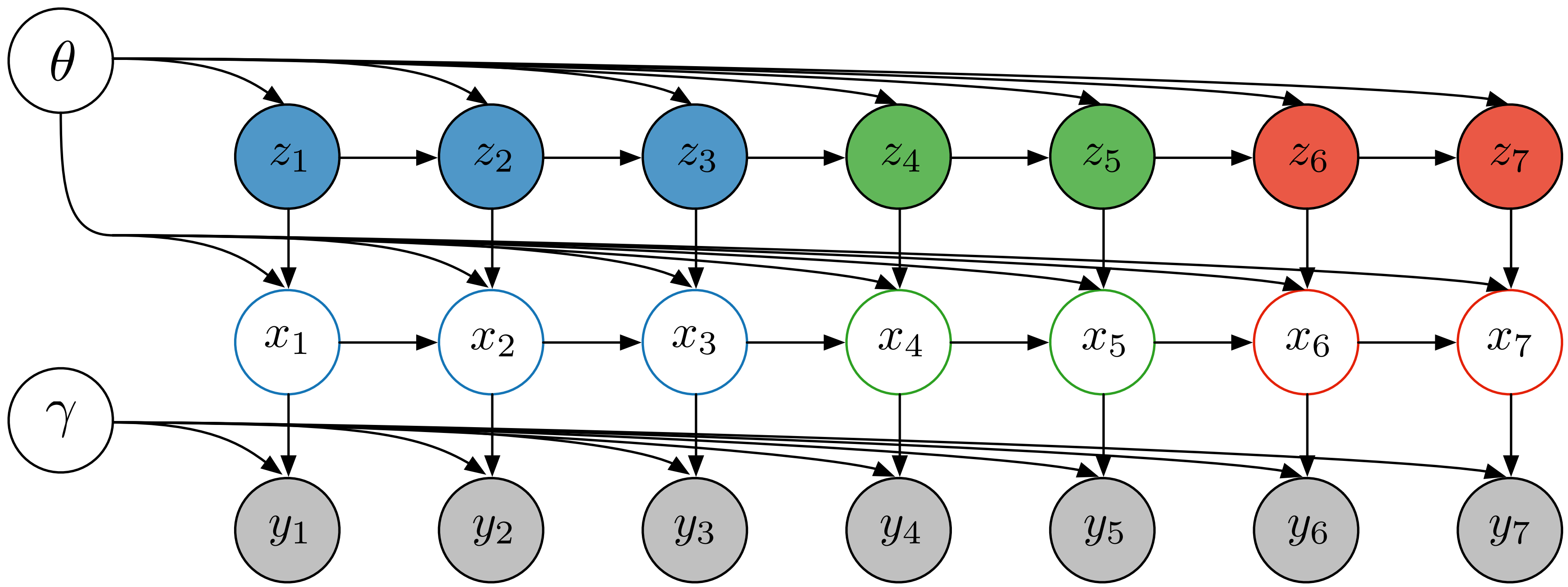
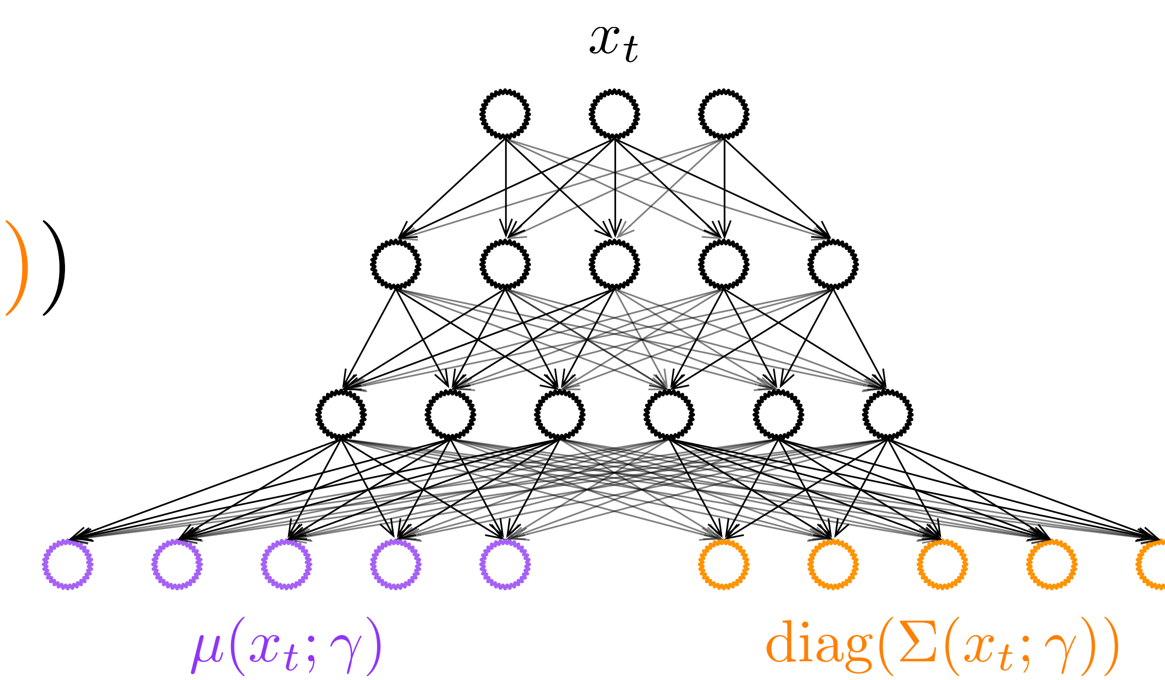
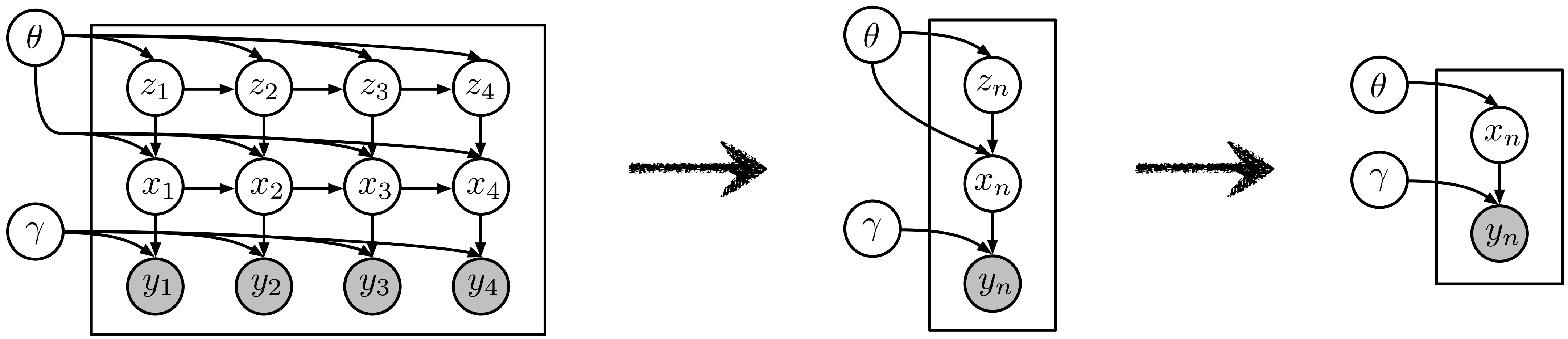
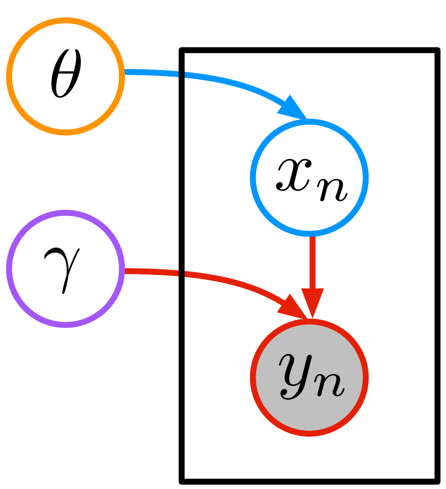


$$y_t \,|\, x_t, \gamma \;\sim\; \mathcal{N}(\mu(x_t; \gamma), \Sigma(x_t; \gamma))$$





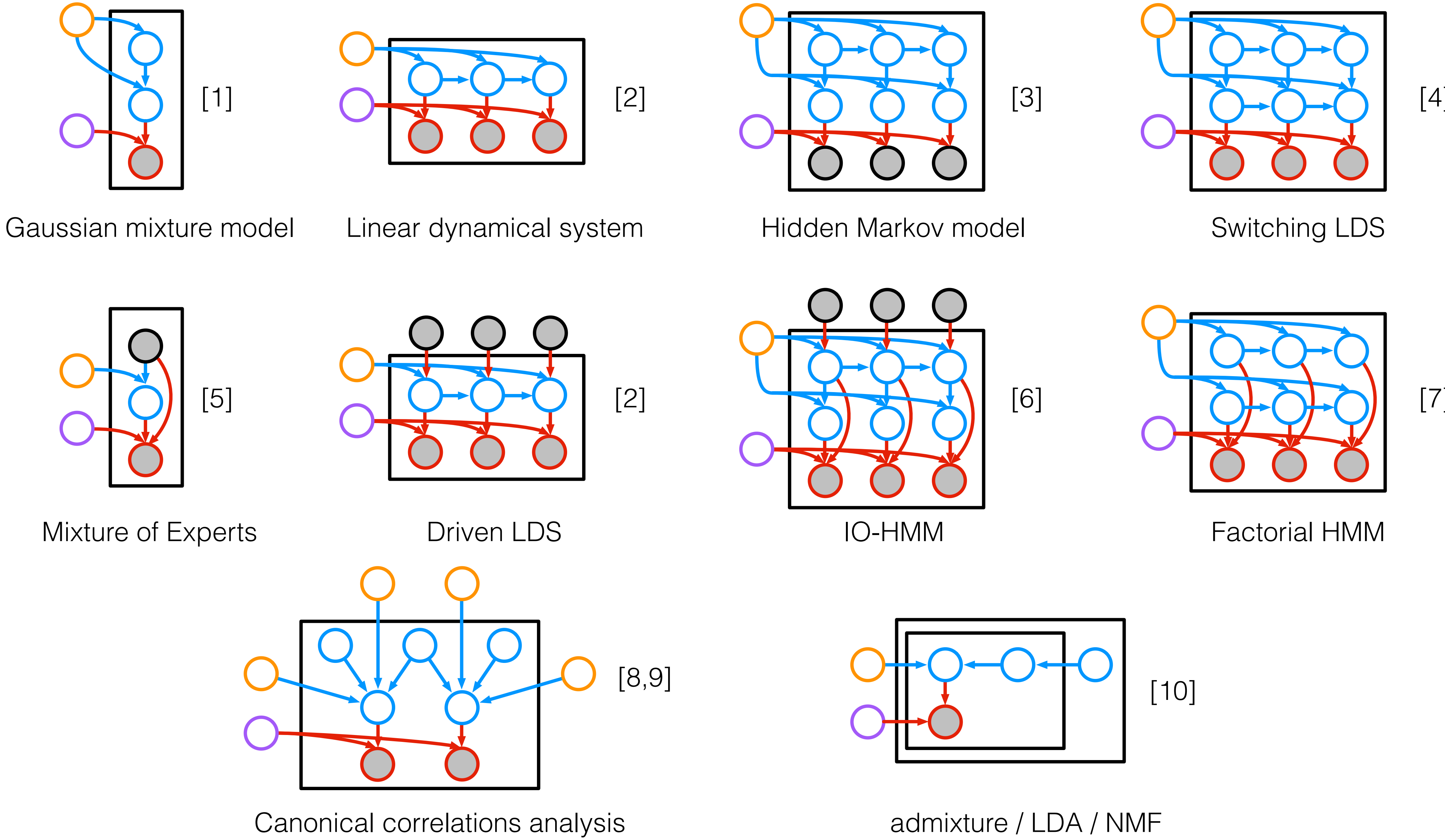


$p(\theta)$ conjugate prior on global variables

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

$p(\gamma)$ any prior on observation parameters

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



[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.
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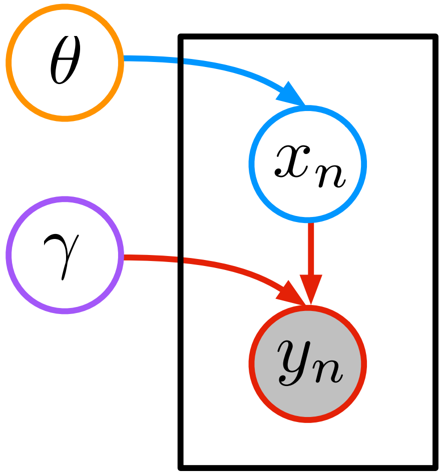
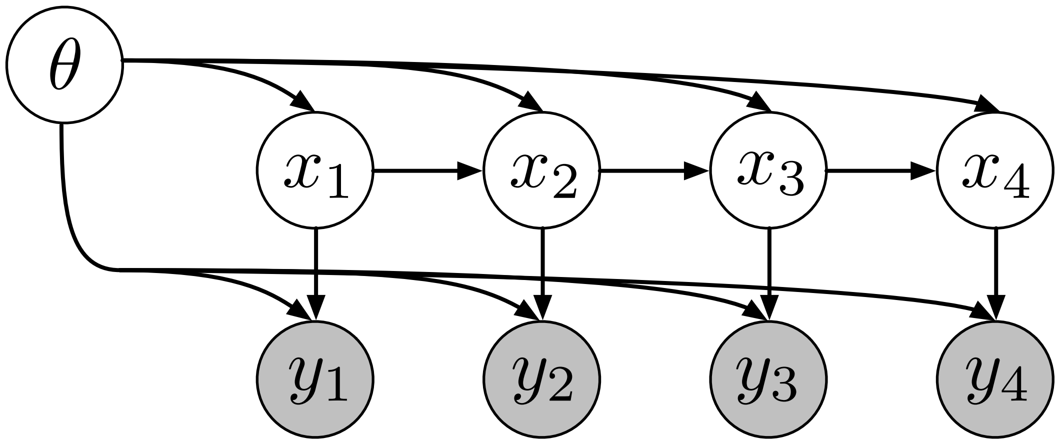
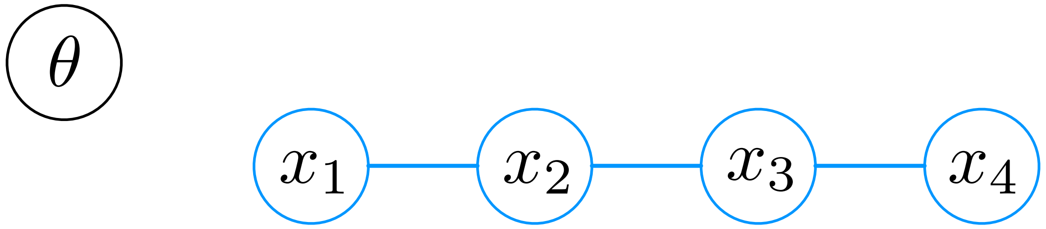


Inference?



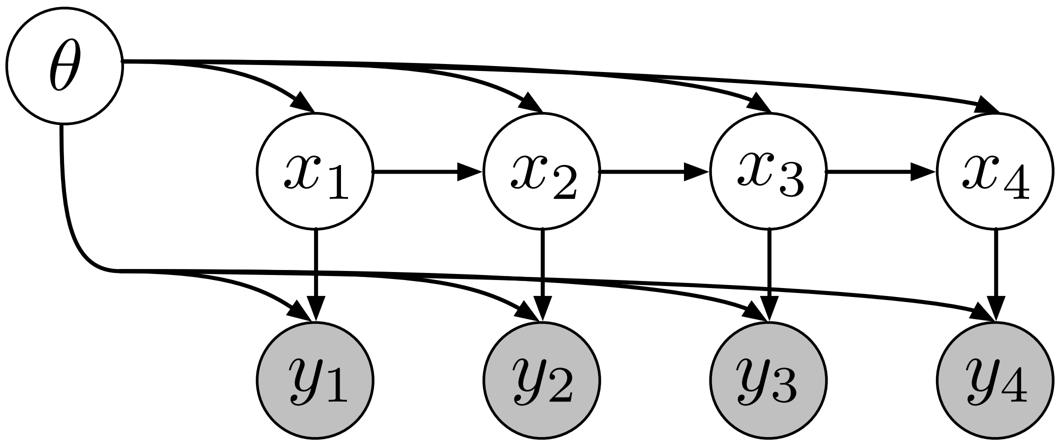


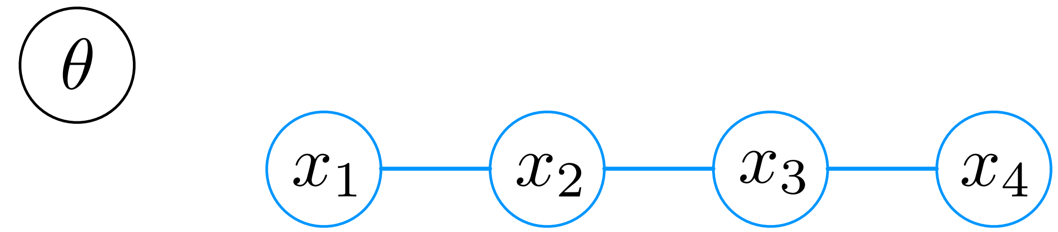
$p(x \,|\, \theta)$ is linear dynamical system
$p(y \,|\, x, \theta)$ is linear-Gaussian
$p(\theta)$ is conjugate prior

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

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

$$q(\theta) \leftrightarrow \eta_\theta \qquad q(x) \leftrightarrow \eta_x$$





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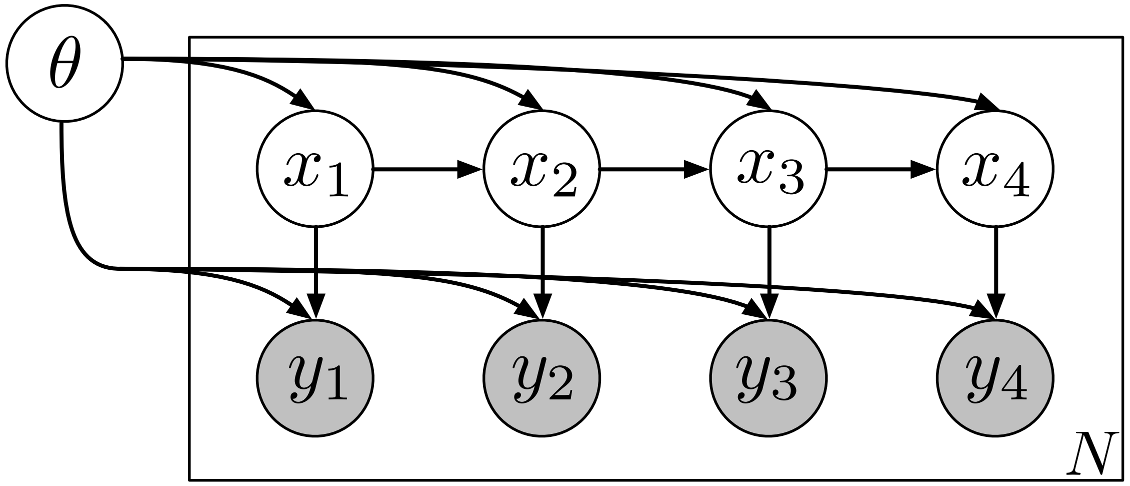
$$q(\theta)q(x) \approx p(\theta, x \mid y)$$

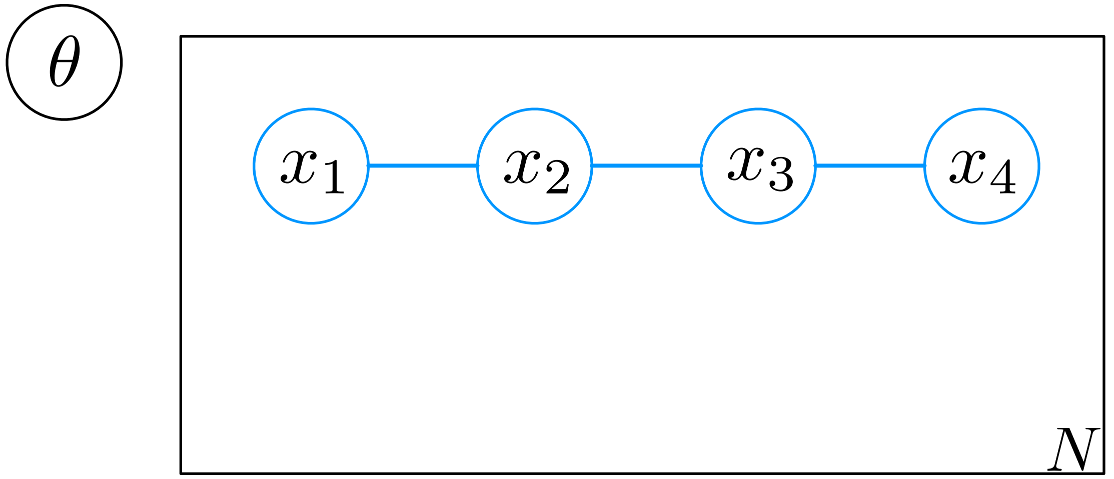
$$\mathcal{L}(\eta_\theta, \eta_x) \triangleq \mathbb{E}_{q(\theta)q(x)}\left[\log \frac{p(\theta, x, y)}{q(\theta)q(x)}\right]$$

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

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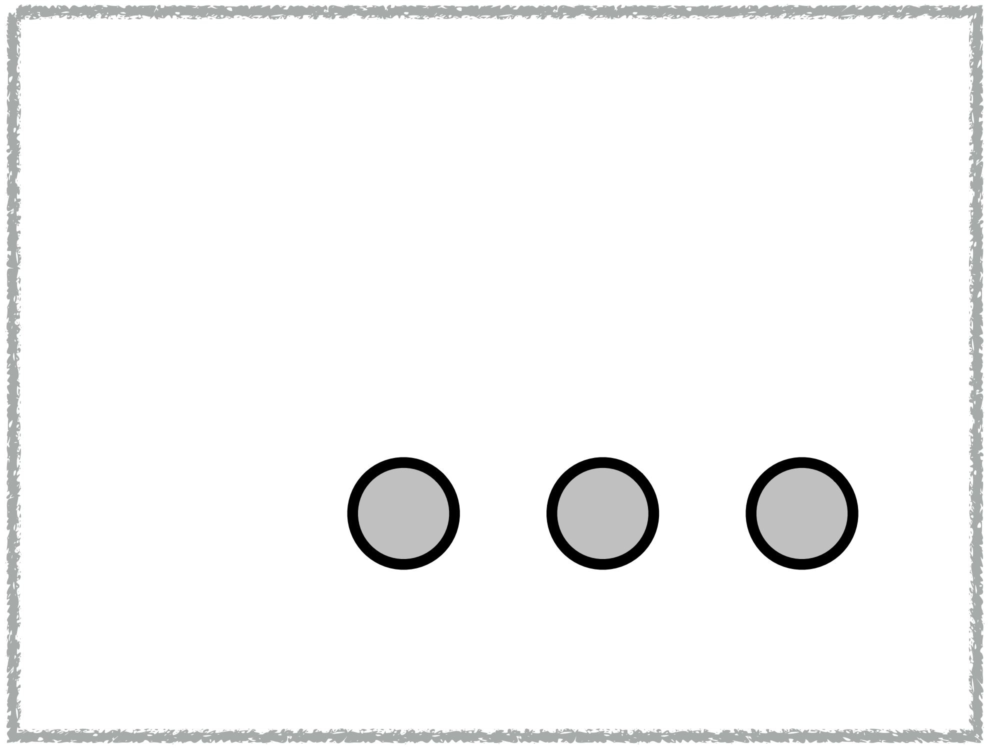
Proposition (natural gradient SVI of Hoffman et al. 2013)

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

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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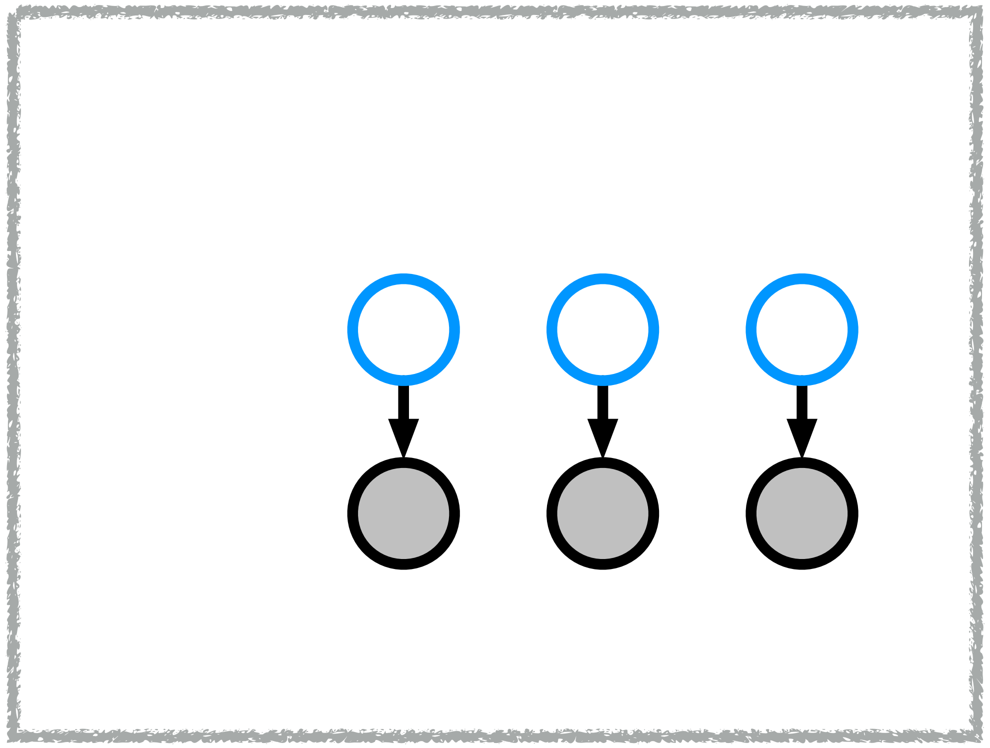

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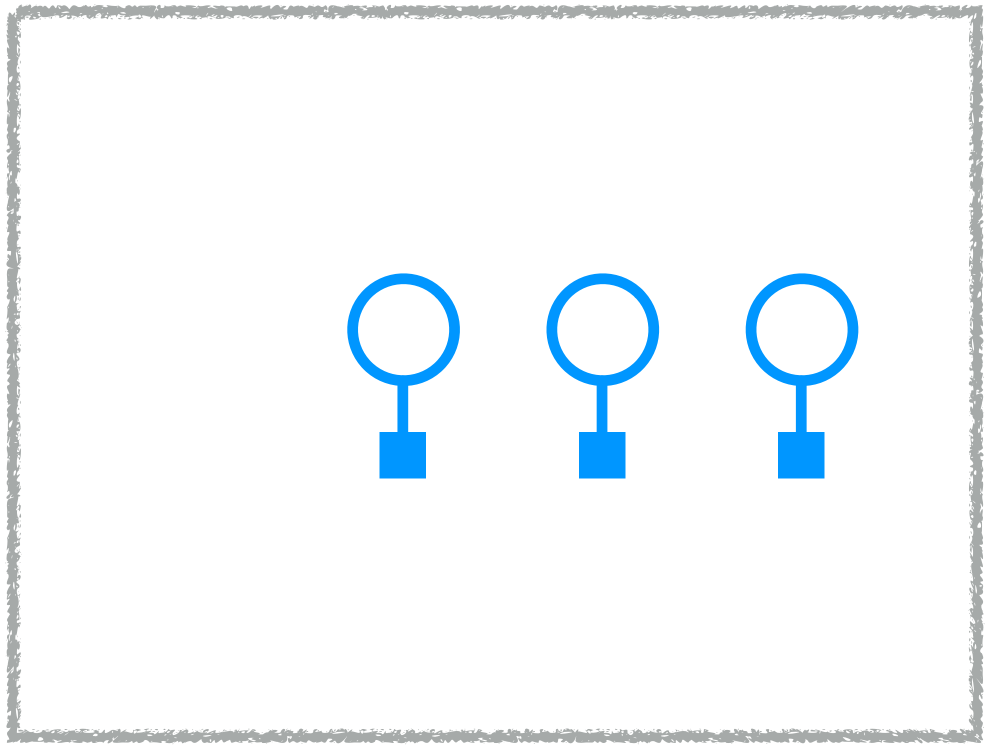
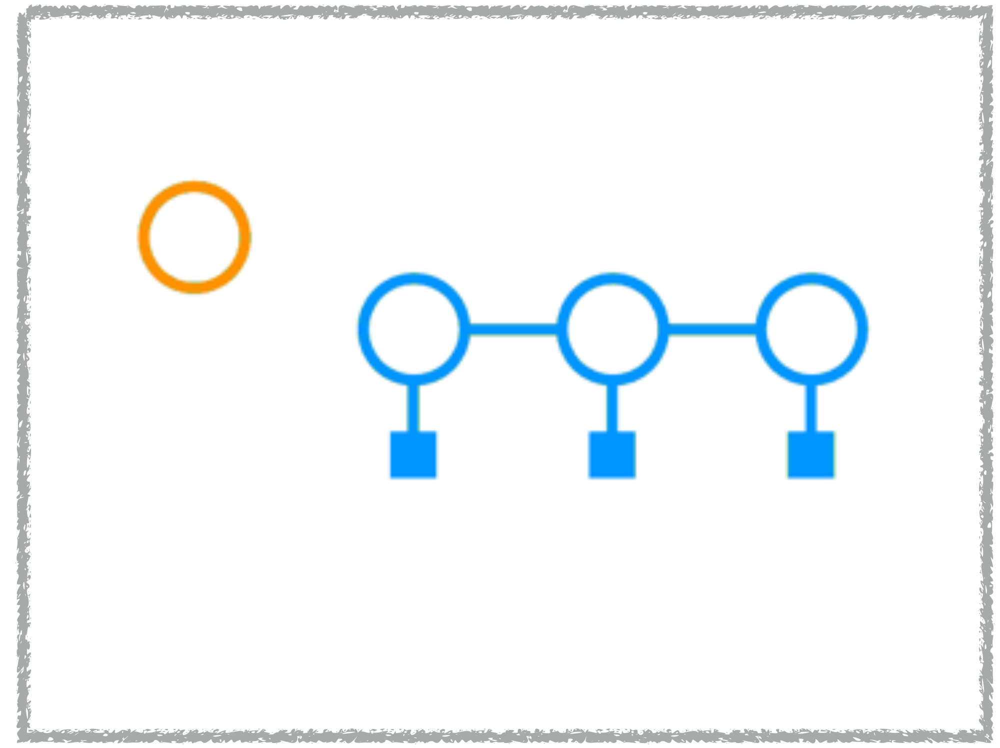
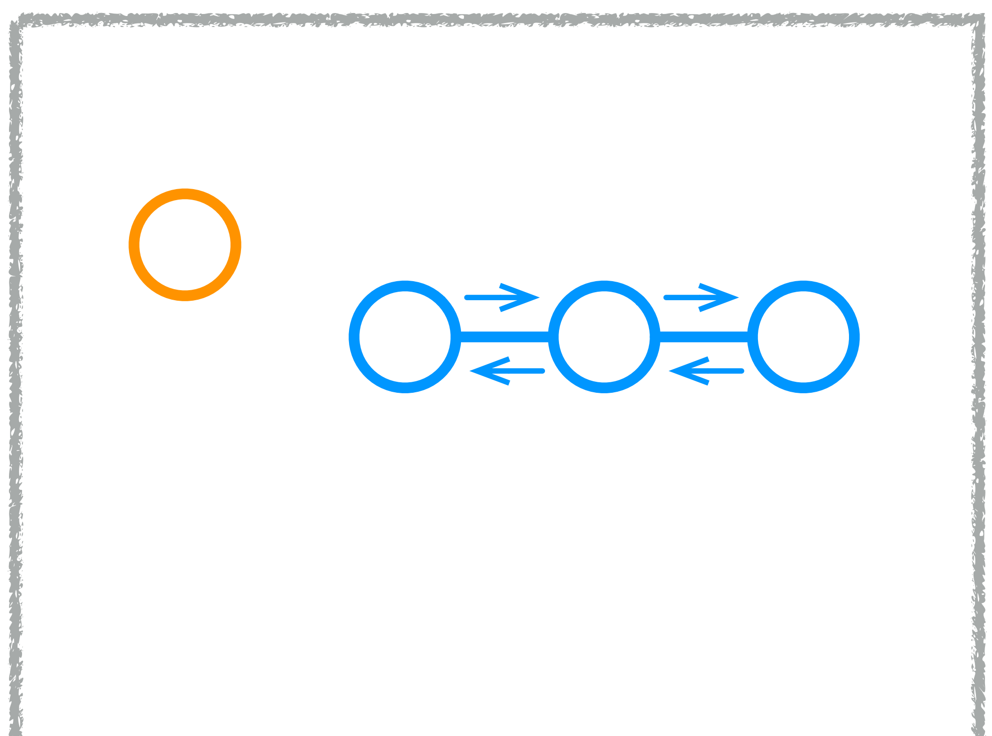


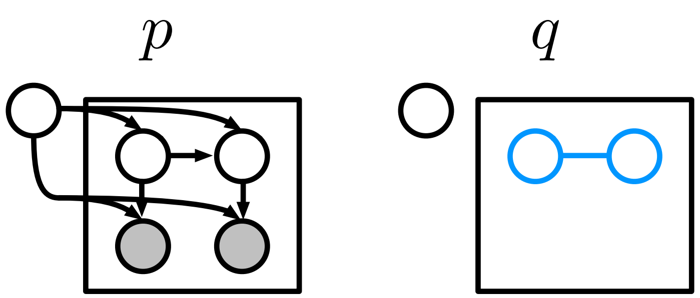
Step 2: run fast message passing

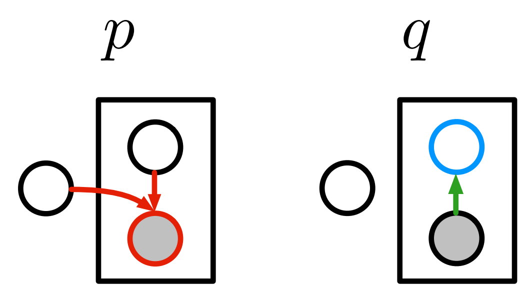


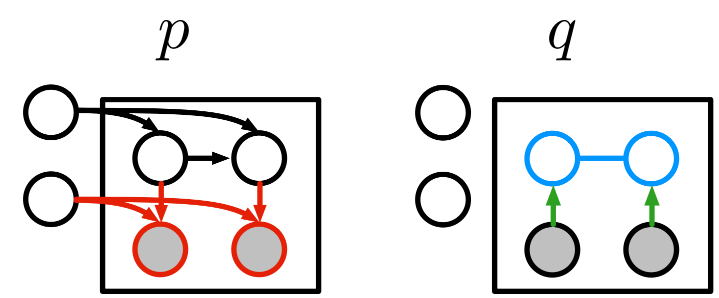
Step 3: compute natural gradient



[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.







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

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

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

Natural gradient SVI

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

Variational autoencoders [1,2]

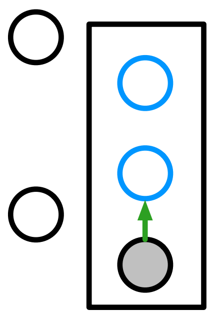
– suboptimal local factor
+ fast for general obs.
– ϕ does all local inference
– no natural gradients

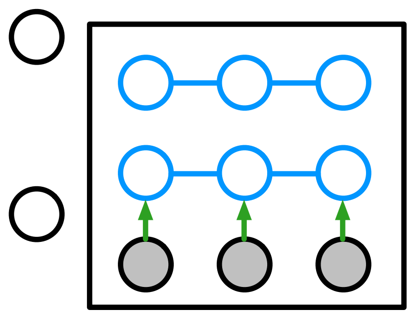
Structured VAEs

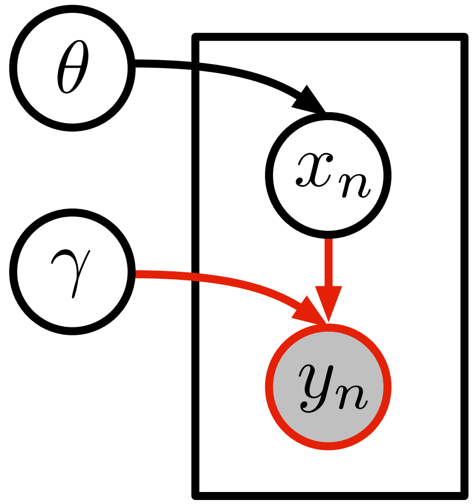
± optimal given conj. evidence
+ fast for general obs.
+ exploits conj. graph structure
+ natural gradients on η_θ

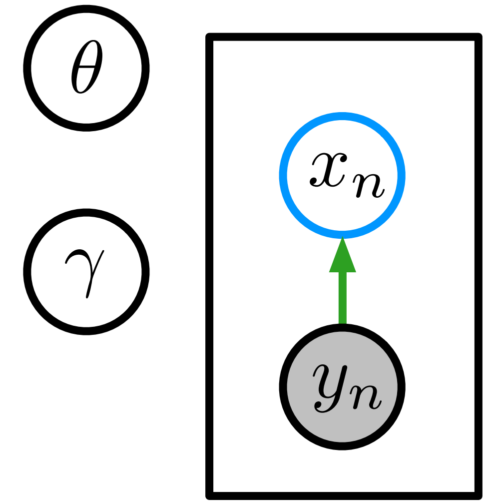
[1] Kingma and Welling. Auto-encoding variational Bayes. ICLR 2014.
[2] Rezende, Mohamed, and Wierstra. Stochastic backpropagation and approximate inference in deep generative models. ICML 2014

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



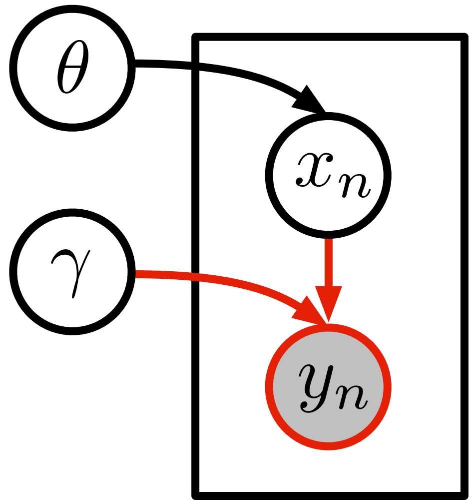


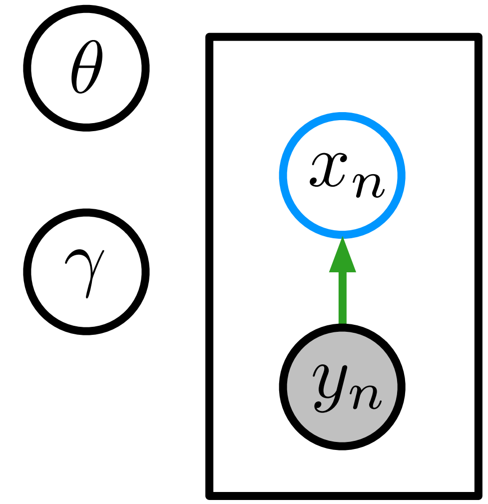




$$\mathcal{L}[\,q(\theta)q(\gamma)q(x)\,] \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)}\left[\log \frac{p(\theta,\gamma,x)p(y\mid x,\gamma)}{q(\theta)q(\gamma)q(x)}\right]$$

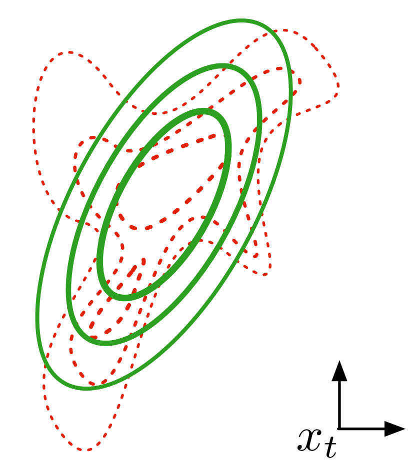
$$q(\theta) \leftrightarrow \eta_\theta \qquad q(\gamma) \leftrightarrow \eta_\gamma \qquad q(x) \leftrightarrow \eta_x$$





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

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



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

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

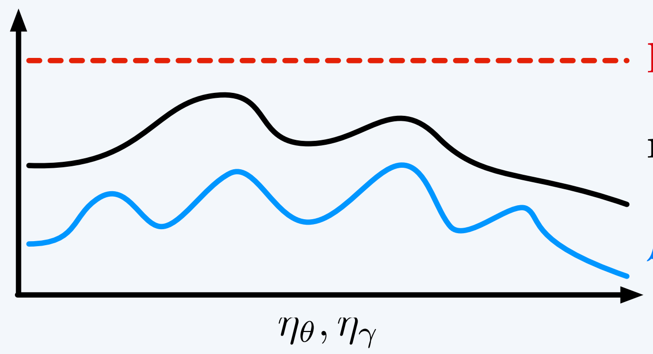
where $\psi(x; y, \phi)$ is a conjugate potential for $p(x \mid \theta)$

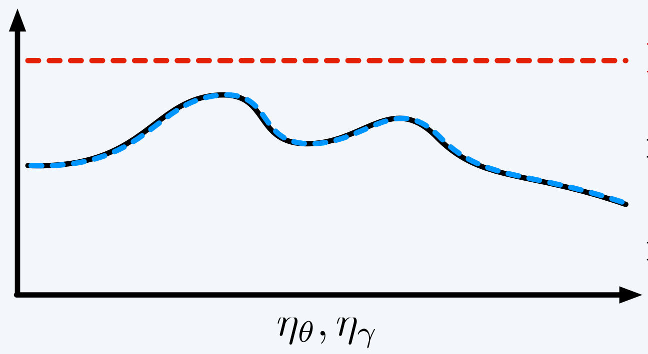
$$\eta_x^*(\eta_\theta, \phi) \triangleq \arg\max_{\eta_x} \widehat{\mathcal{L}}(\eta_\theta, \eta_x, \phi) \qquad \mathcal{L}_{\text{SVAE}}(\eta_\theta, \eta_\gamma, \phi) \triangleq \mathcal{L}(\eta_\theta, \eta_\gamma, \eta_x^*(\eta_\theta, \phi))$$

Fact (conjugate graphical models are easy)

The local variational parameter $\eta_x^*(\eta_\theta, \phi)$ is easy to compute.

Proposition (log evidence lower bound)





if $\exists\, \phi \in \mathbb{R}^m$ with $\psi(x; y, \phi) = \mathbb{E}_{q(\gamma)} \log p(y \,|\, x, \gamma)$

Proposition (reparameterization trick)

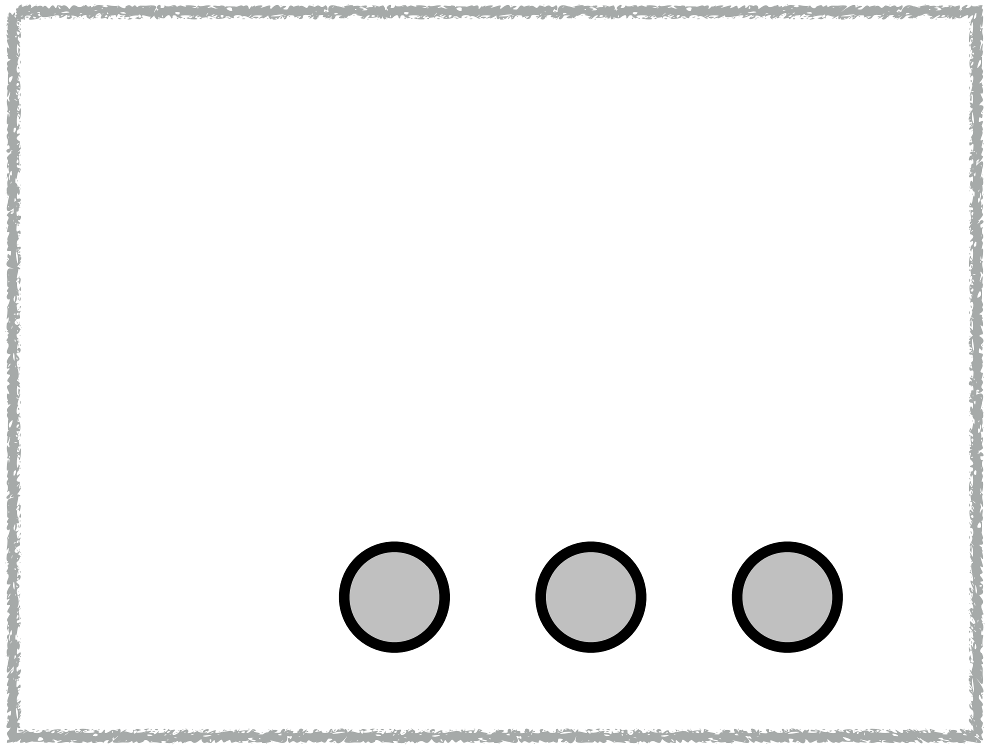
Estimate $\nabla_{\eta_\gamma, \phi} \mathcal{L}_{\mathrm{SVAE}}(\eta_\theta, \eta_\gamma, \phi)$ with samples $\hat{\gamma} \sim q(\gamma)$ and $\hat{x} \sim q^*(x \,|\, \phi)$ via

$$\mathcal{L}_{\mathrm{SVAE}}(\eta_\theta, \eta_\gamma, \phi) \approx \log p(y \,|\, \hat{x}, \hat{\gamma}) - \mathrm{KL}(q(\theta) q(\gamma) q^*(x \,|\, \phi) \,\|\, p(\theta, \gamma, x))$$

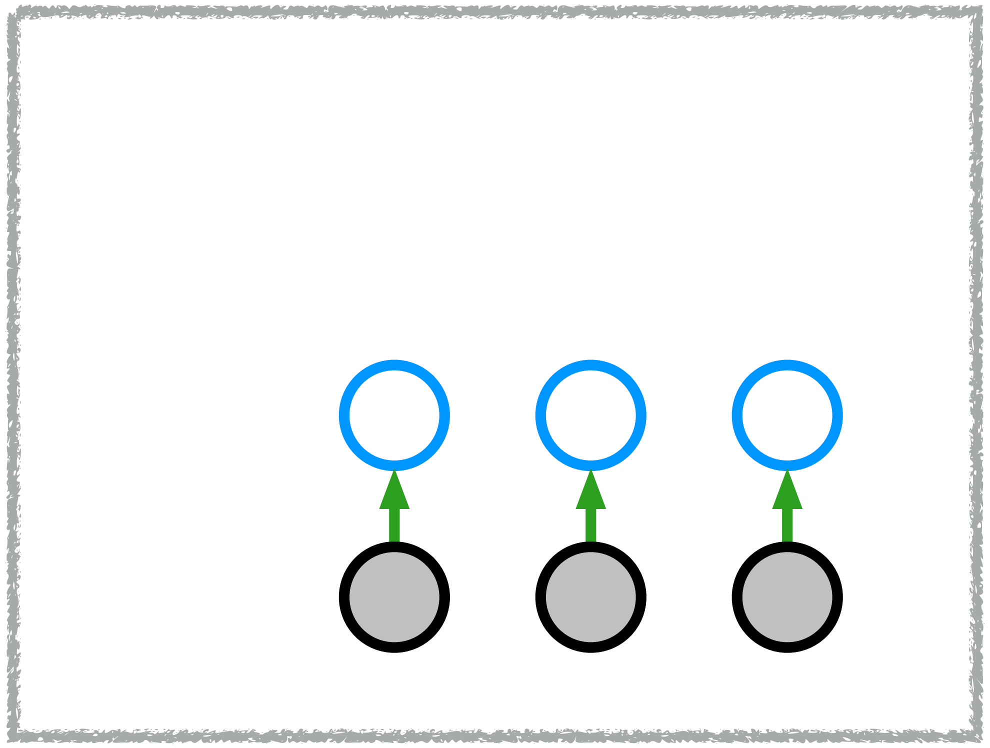
Proposition (easy natural gradient)

$$\widetilde{\nabla}_{\eta_\theta} \mathcal{L}_{\mathrm{SVAE}}(\eta_\theta, \eta_\gamma, \phi) = (\eta_\theta^0 + \mathbb{E}_{q^*(x \,|\, \phi)}(t_x(x), 1) - \eta_\theta) + (\nabla_{\eta_x} \mathcal{L}(\eta_\theta, \eta_\gamma, \eta_x^*(\eta_\theta, \phi)), 0)$$

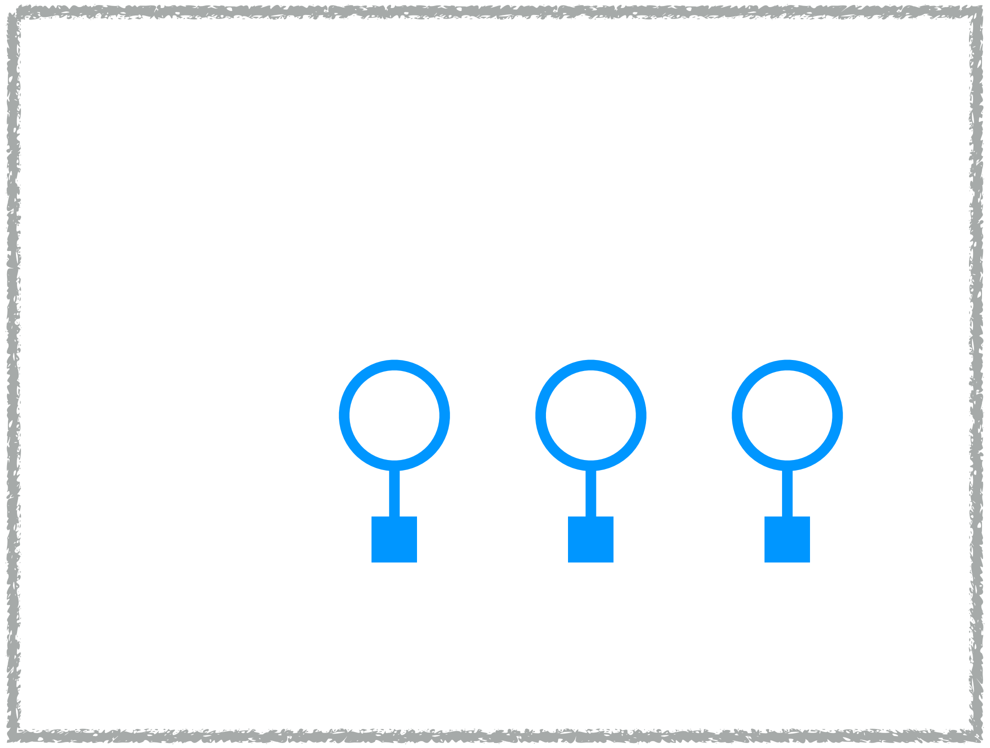
Step 1: apply recognition network



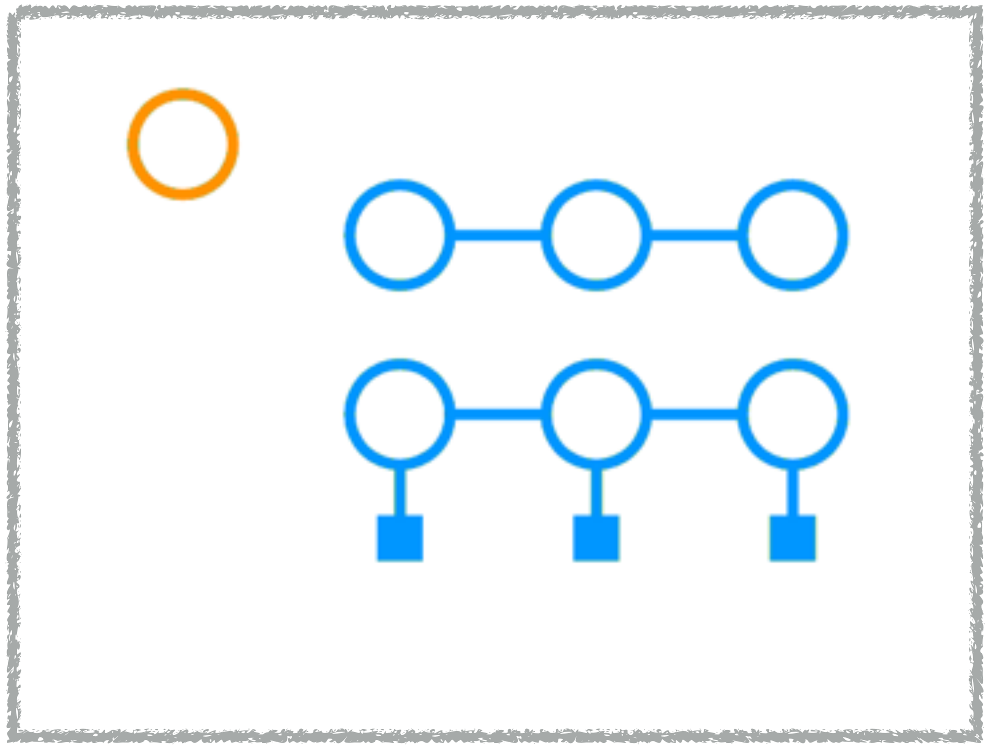
Step 1: apply recognition network



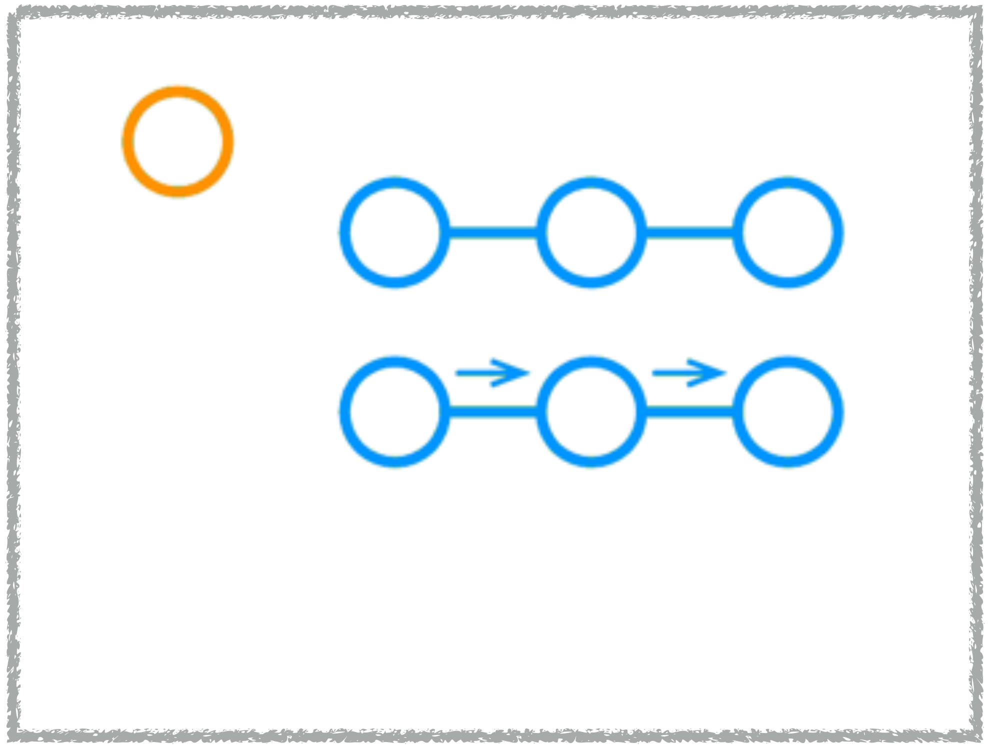
Step 1: apply recognition network



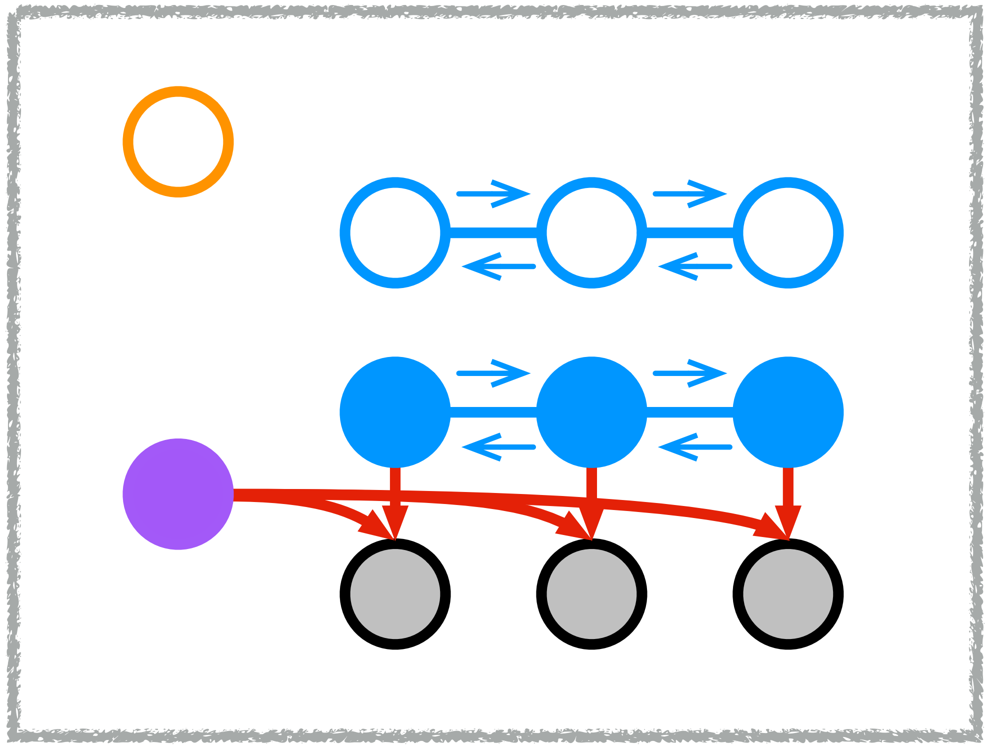
Step 2: run fast PGM algorithms



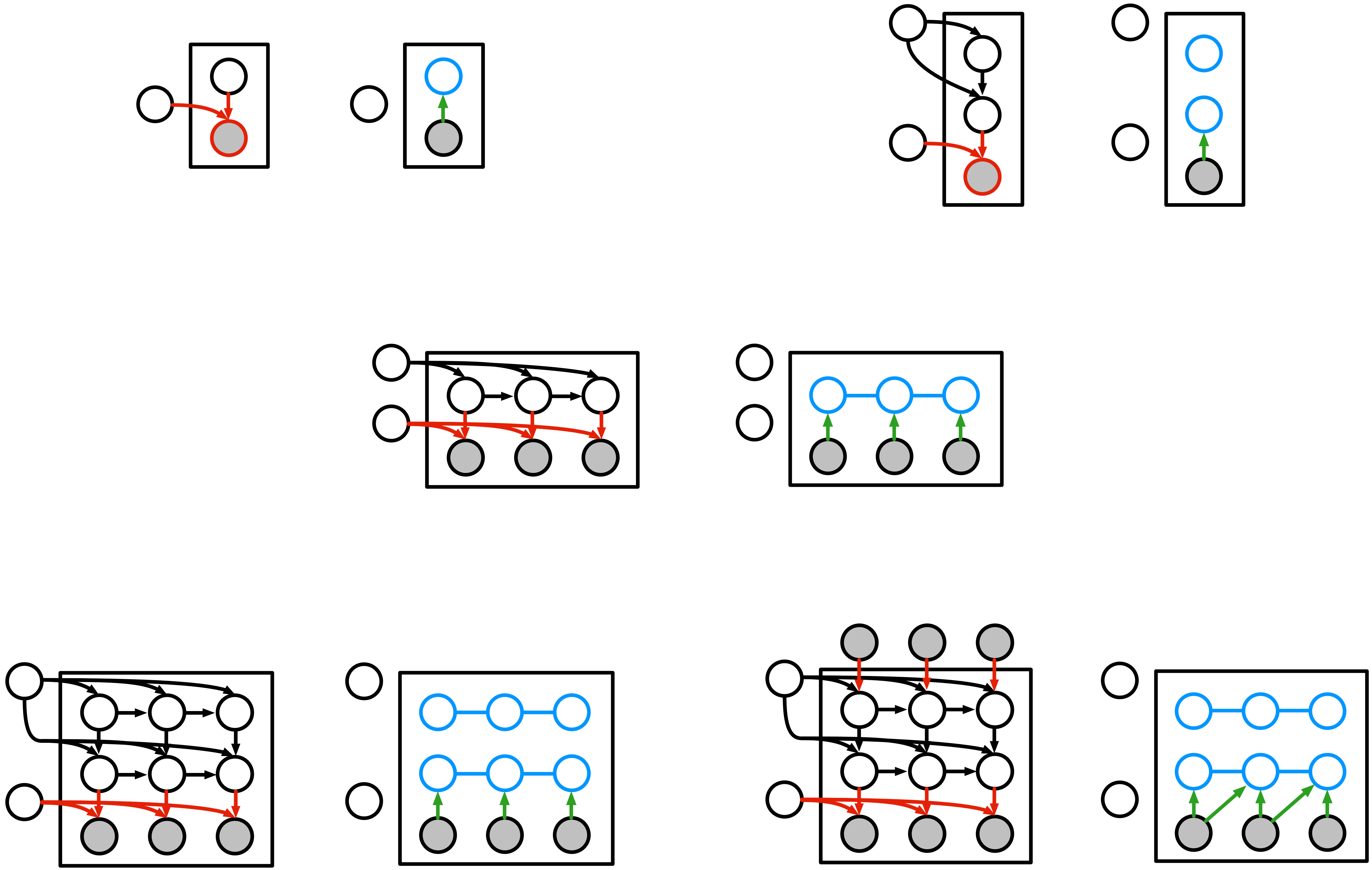
Step 3: sample, compute flat grads

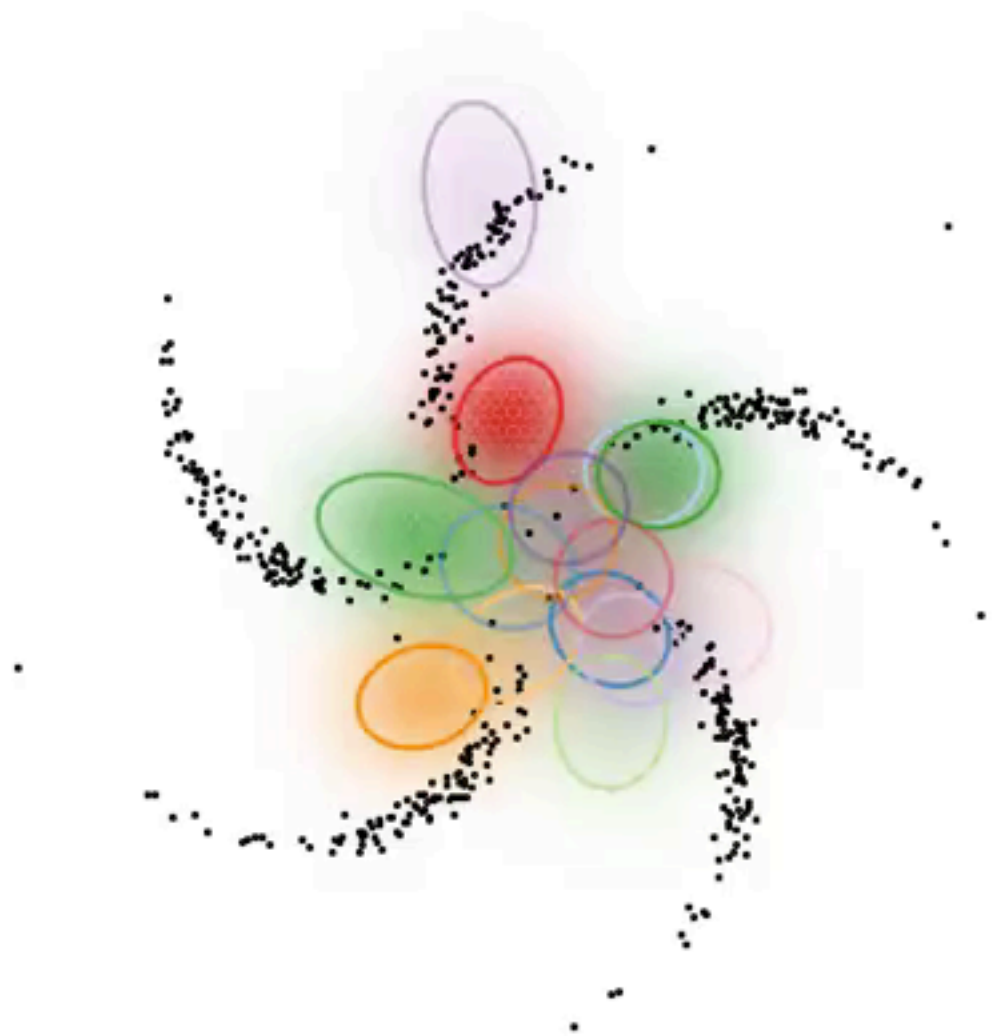


Step 4: compute natural gradient

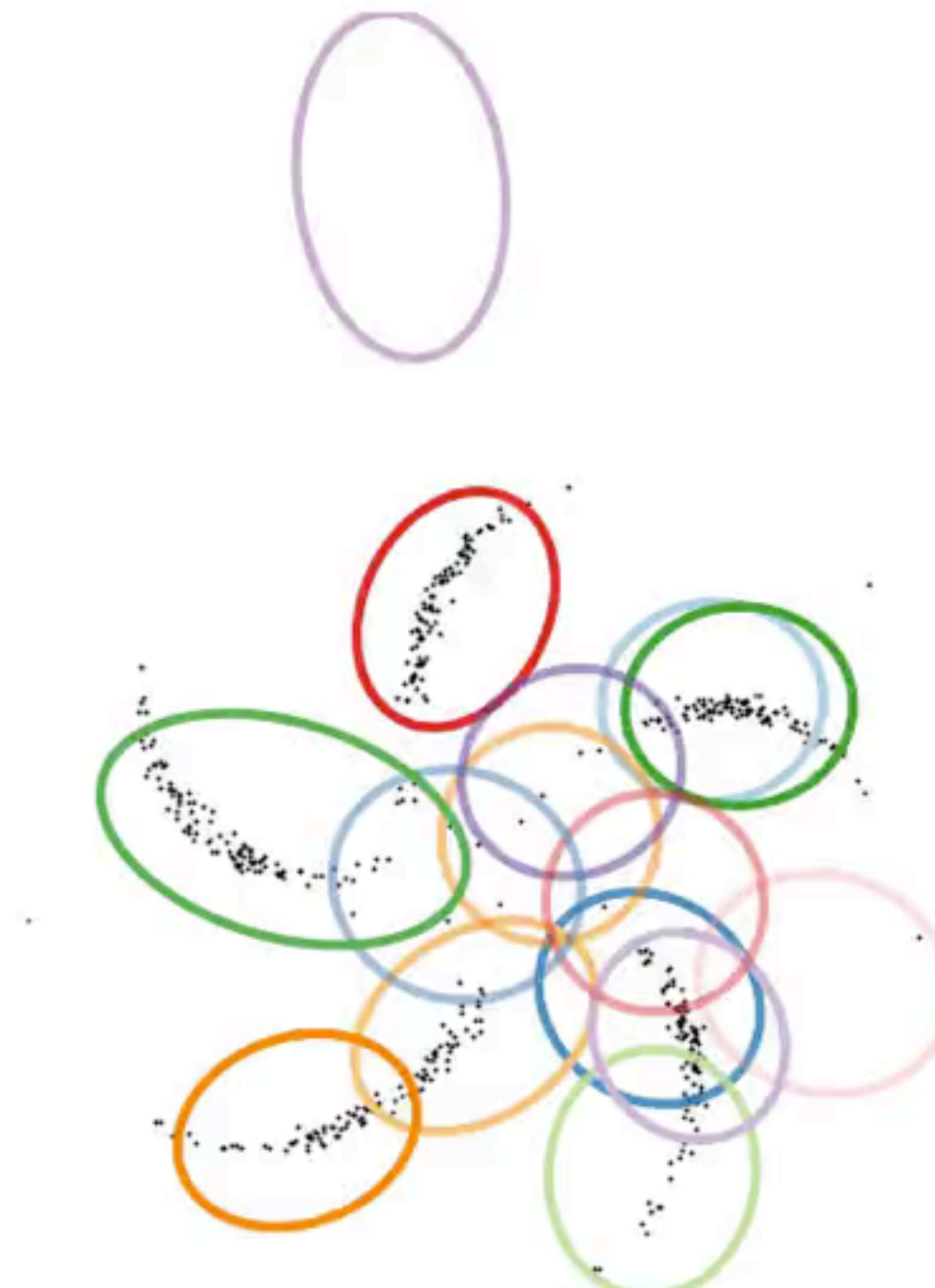


```python
from autograd import value_and_grad as vgrad
from util import add, sub, scale, unbox


def make_gradfun(run_inference, recognize, loglike, eta_prior, return_flat=False):
    saved = lambda: None

    def mc_vlb(eta, gamma, phi, y_n, N, L):
        T = y_n.shape[0]
        nn_potentials = recognize(y_n, phi)
        samples, stats, global_kl, local_kl = run_inference(
            eta_prior, eta, nn_potentials, num_samples=L)
        saved.stats = scale(N, unbox(stats))
        return -global_kl + N * (-local_kl + loglike(y_n, samples, gamma))

    def gradfun(y_n, N, L, eta, gamma, phi):
        objective = lambda (gamma, phi): mc_vlb(eta, gamma, phi, y_n, N, L)
        vlb, (gamma_grad, phi_grad) = vgrad(objective)((gamma, phi))
        eta_natgrad = sub(add(eta_prior, saved.stats), eta)
        return vlb, (eta_natgrad, gamma_grad, phi_grad)

    return gradfun
```

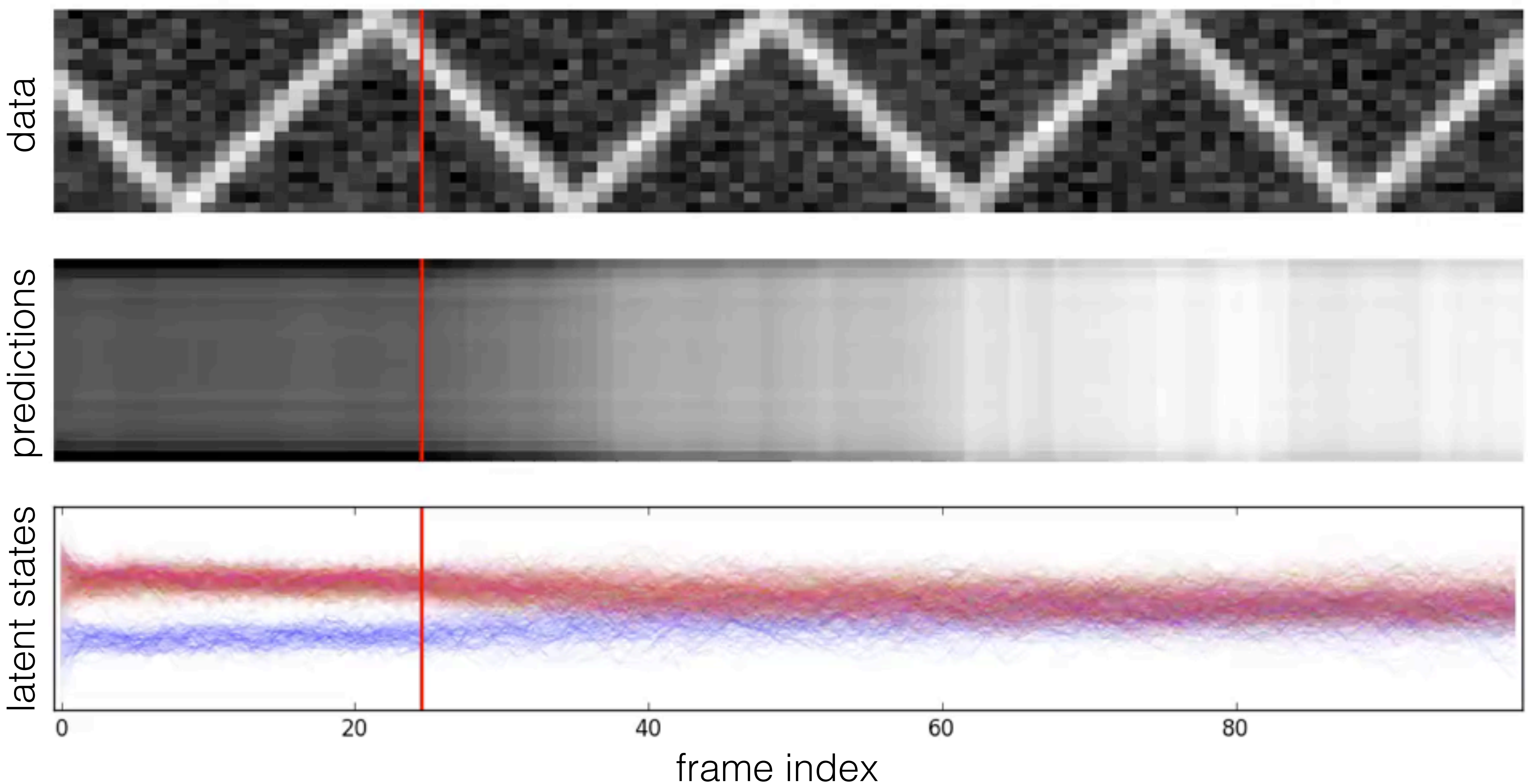




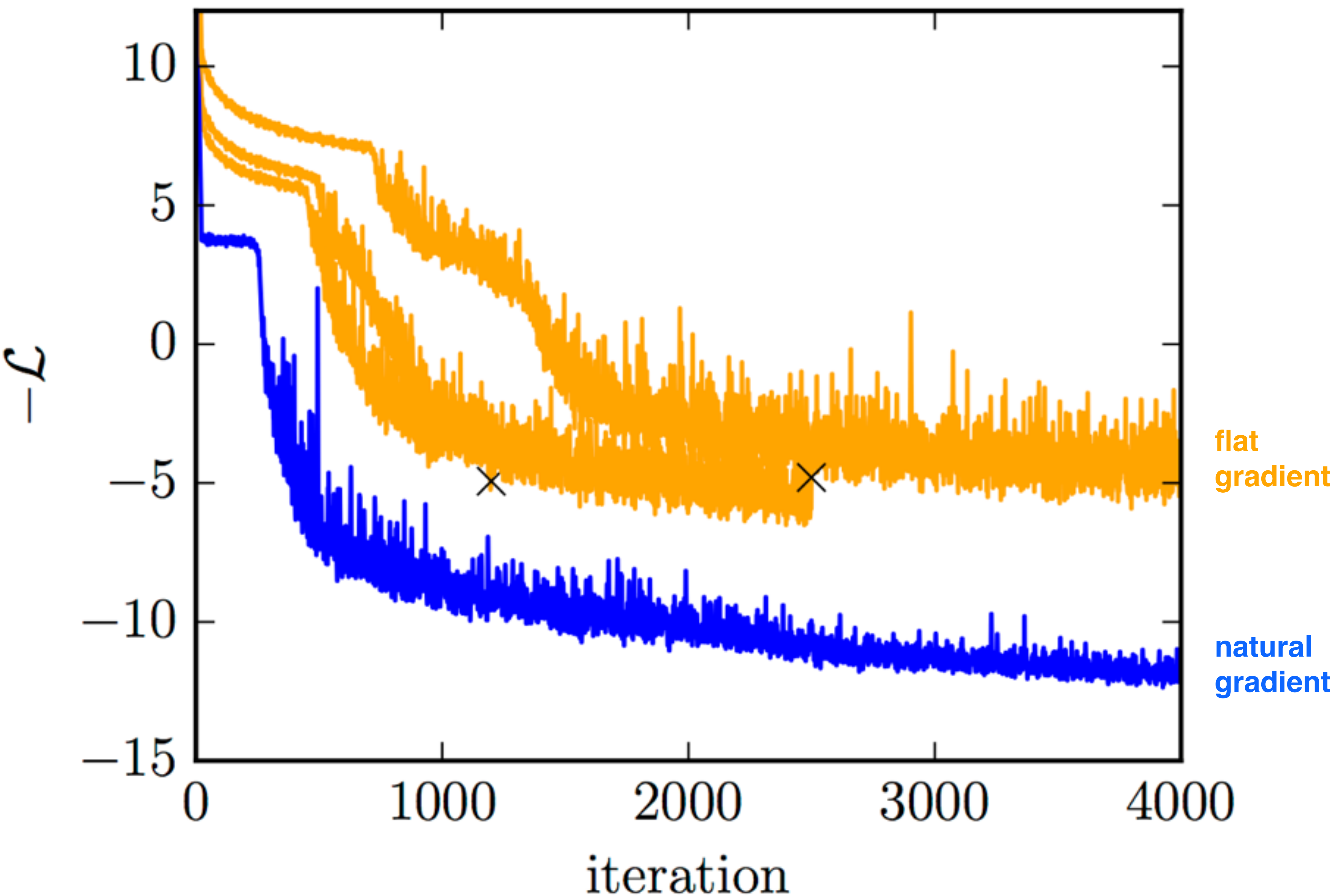
data space



latent space

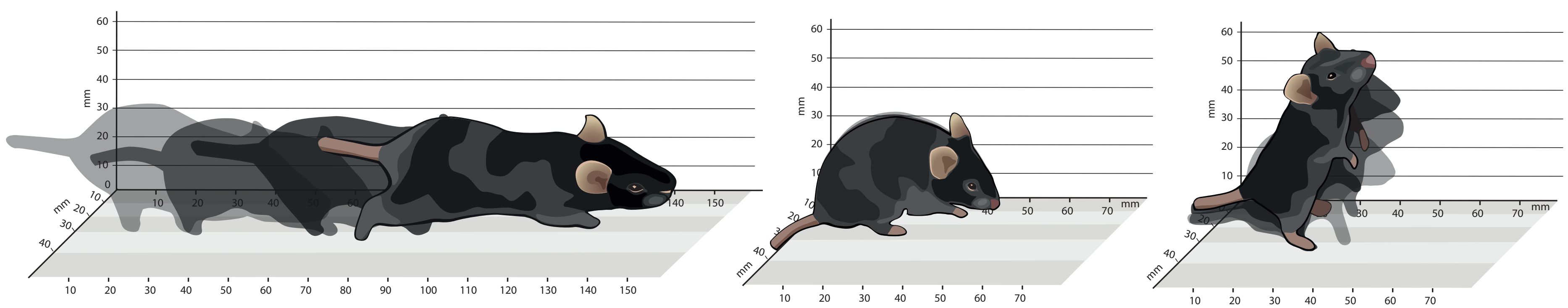


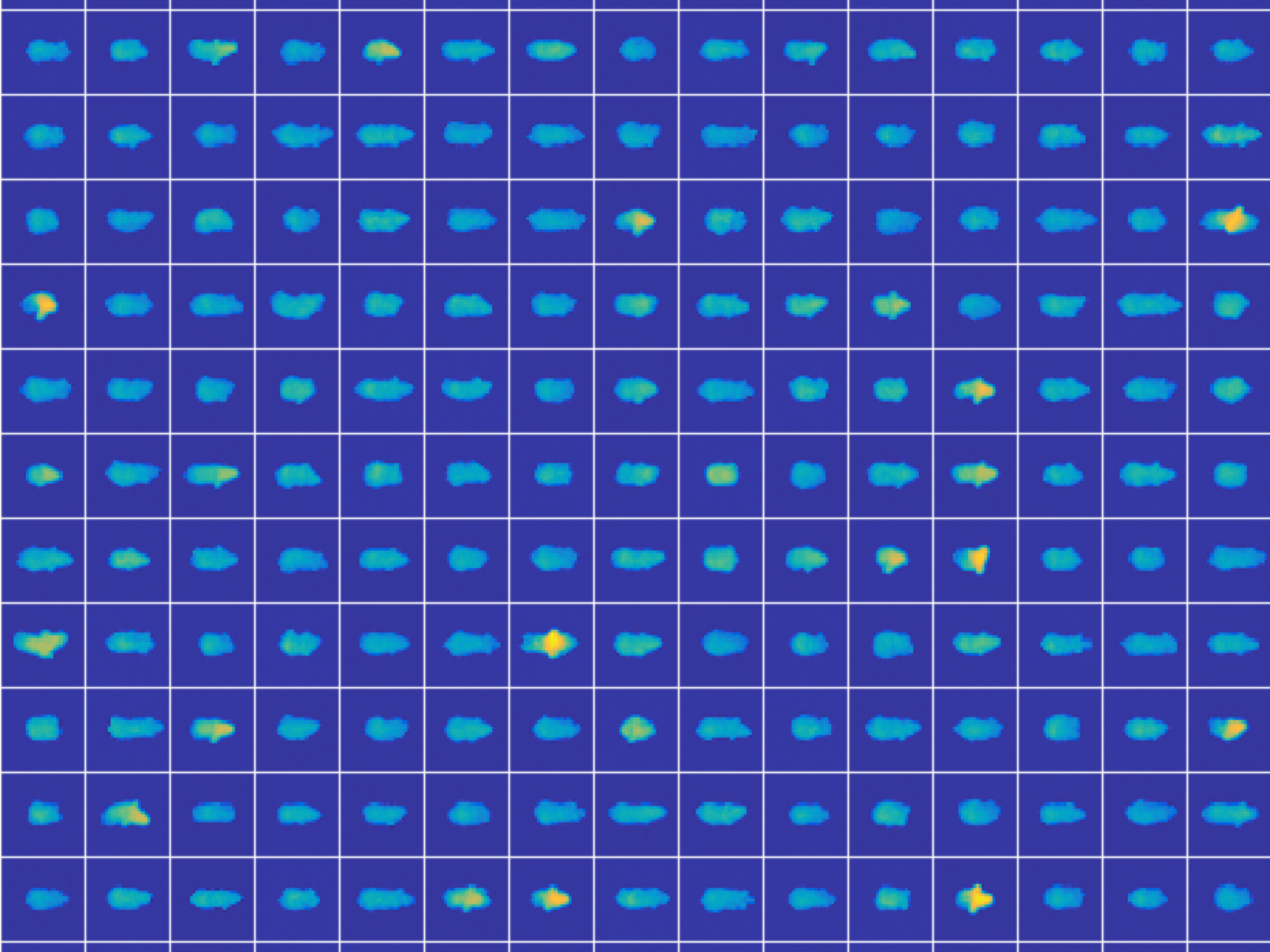
data
predictions
latent states
0
20
40
60
80
frame index

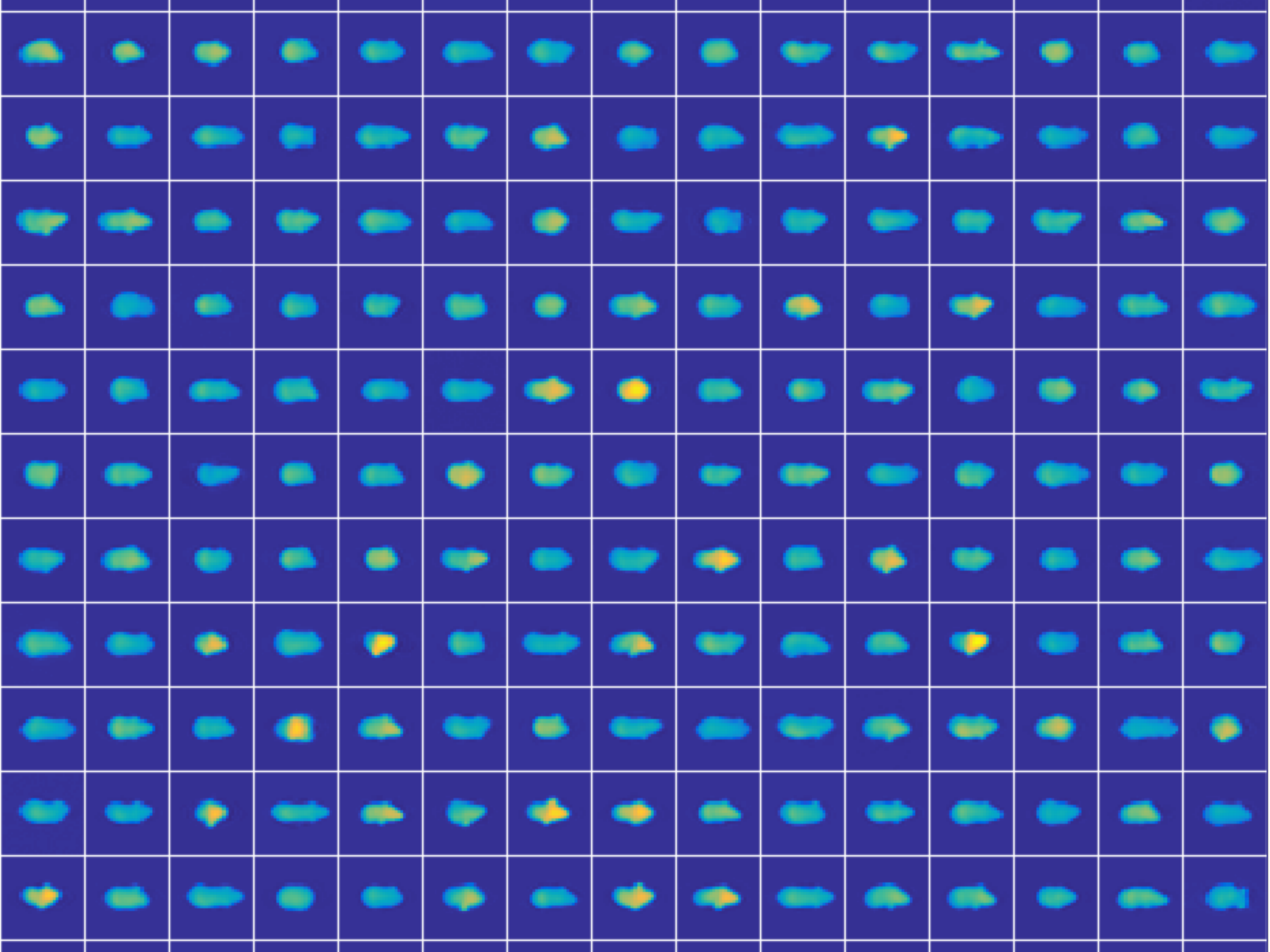


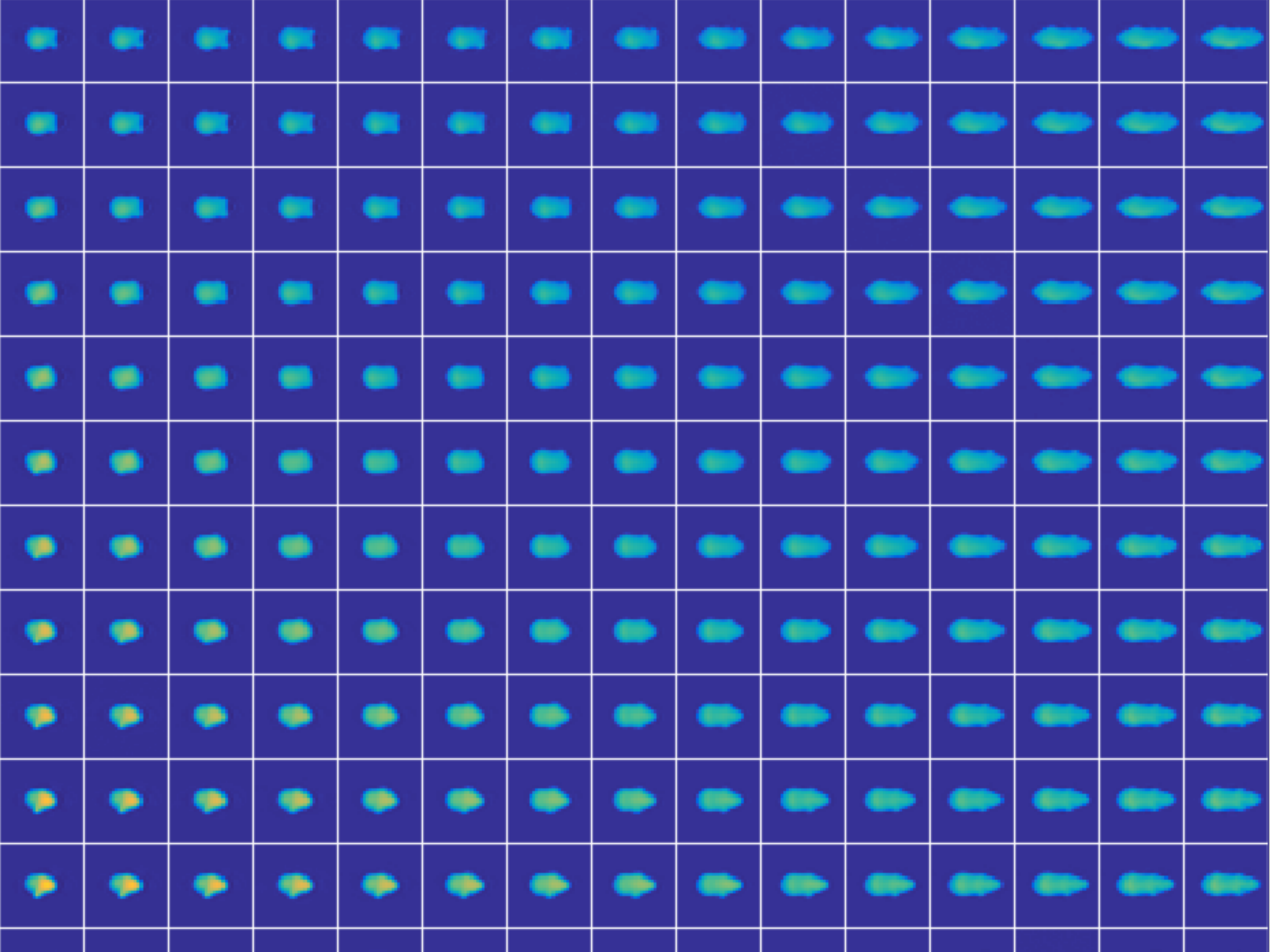
10
5
0
−5
−10
−15
−ℒ
0
1000
2000
3000
4000
iteration
flat
gradient
natural
gradient

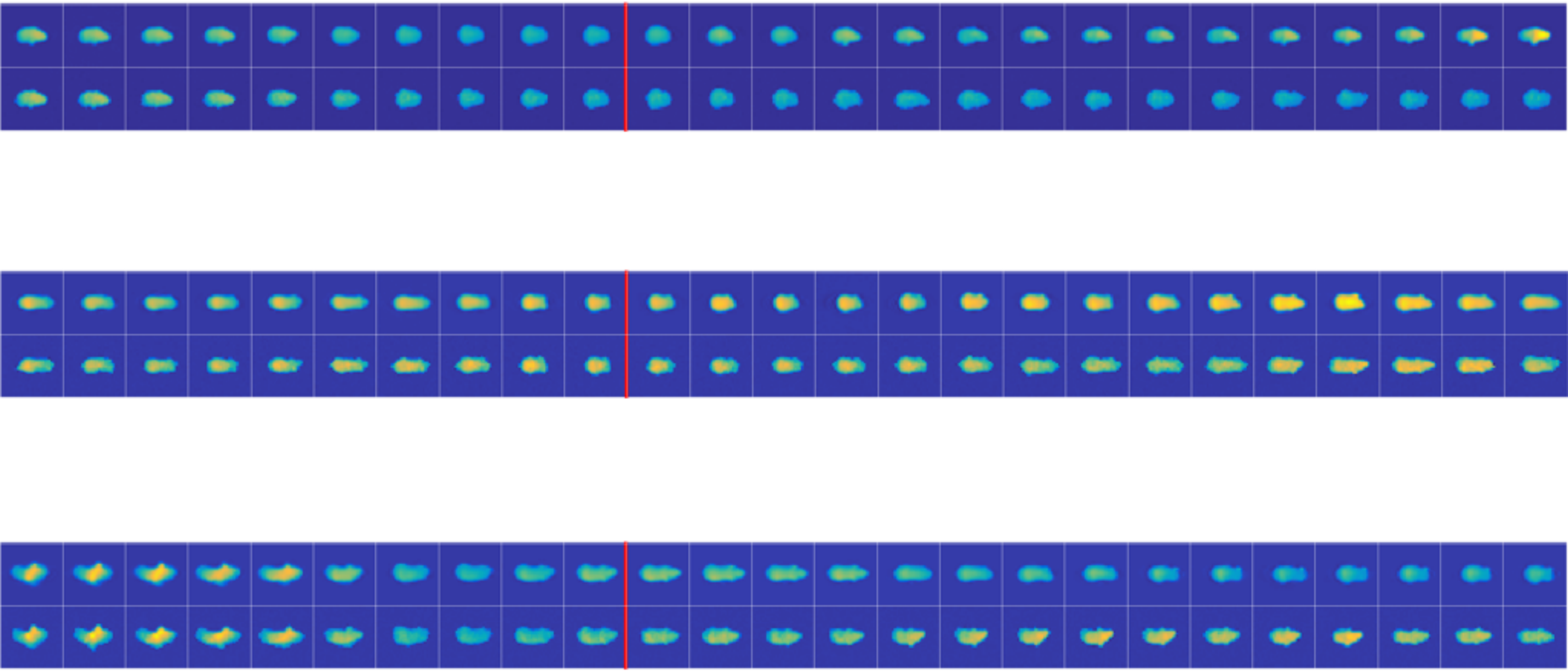
Application: learn syllable representation of behavior from video

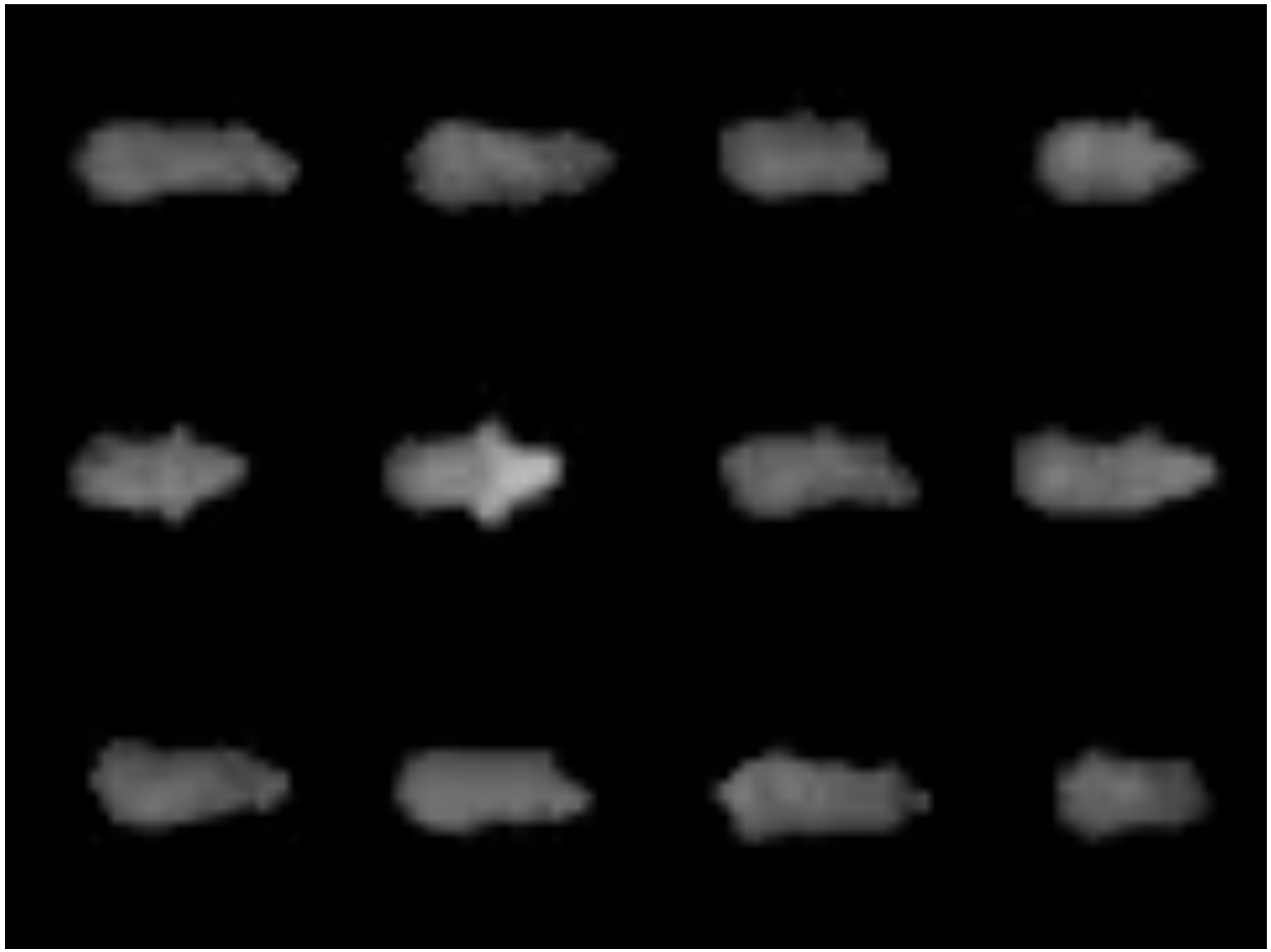




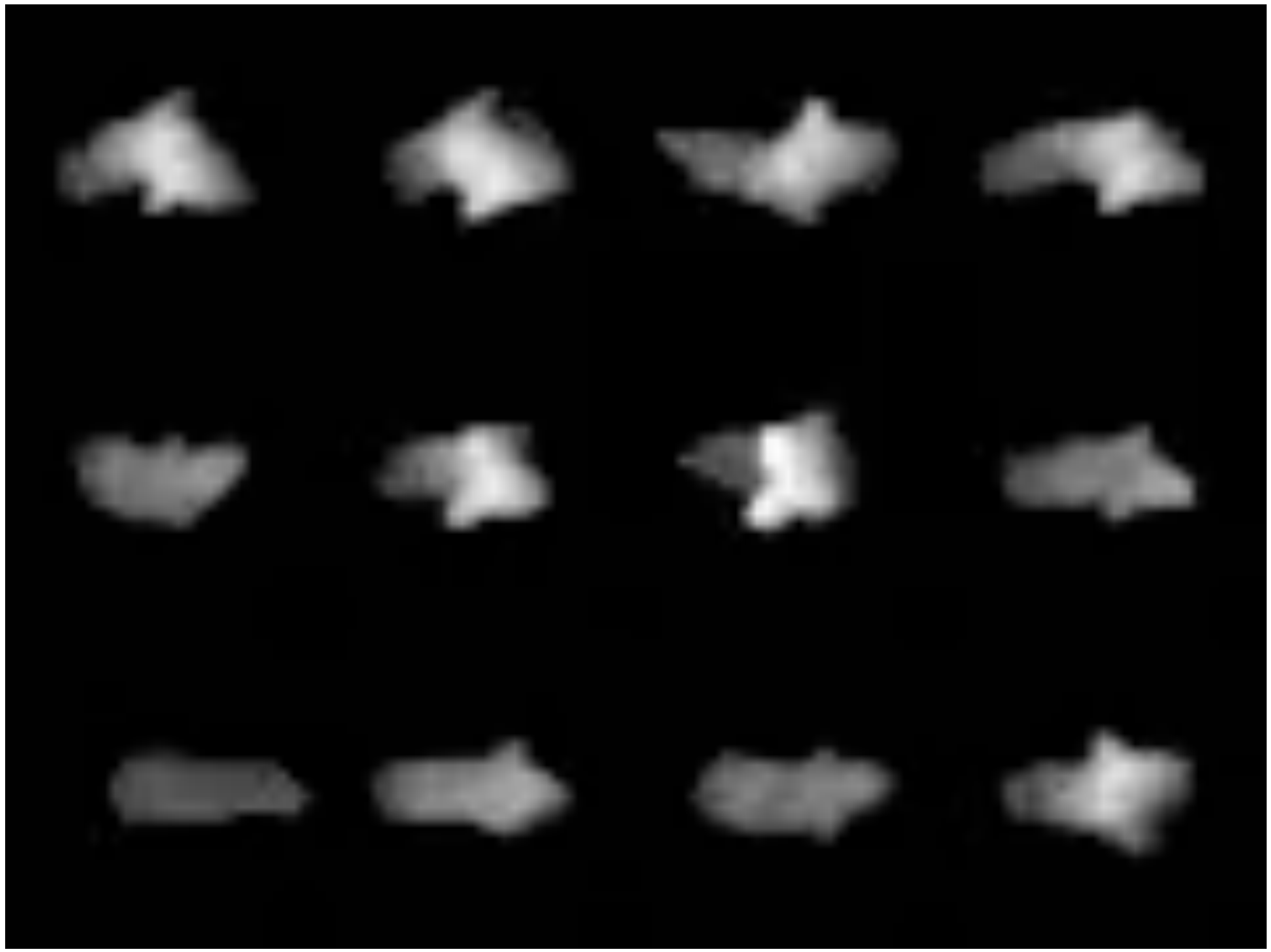




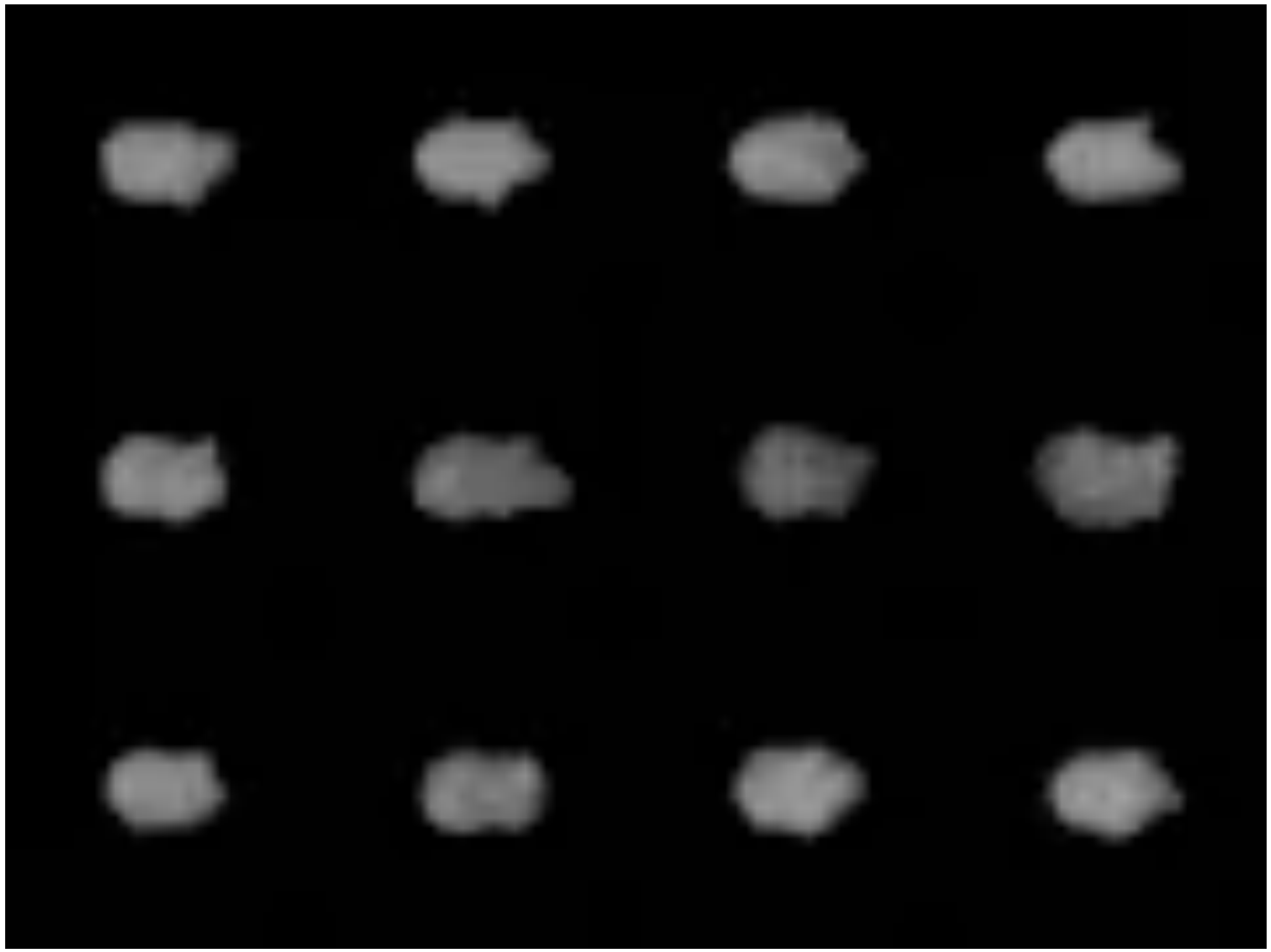




start rear

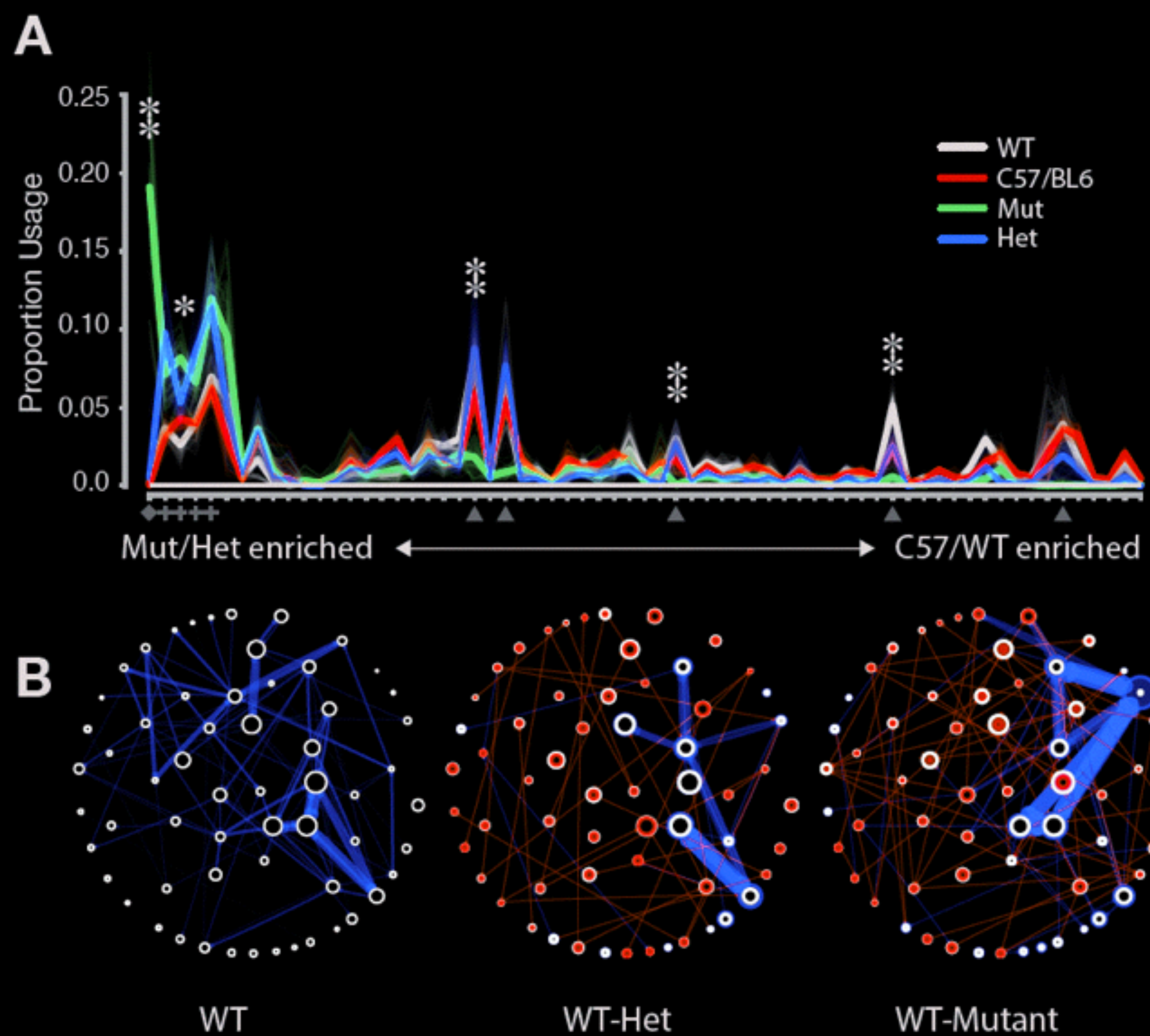


fall from rear



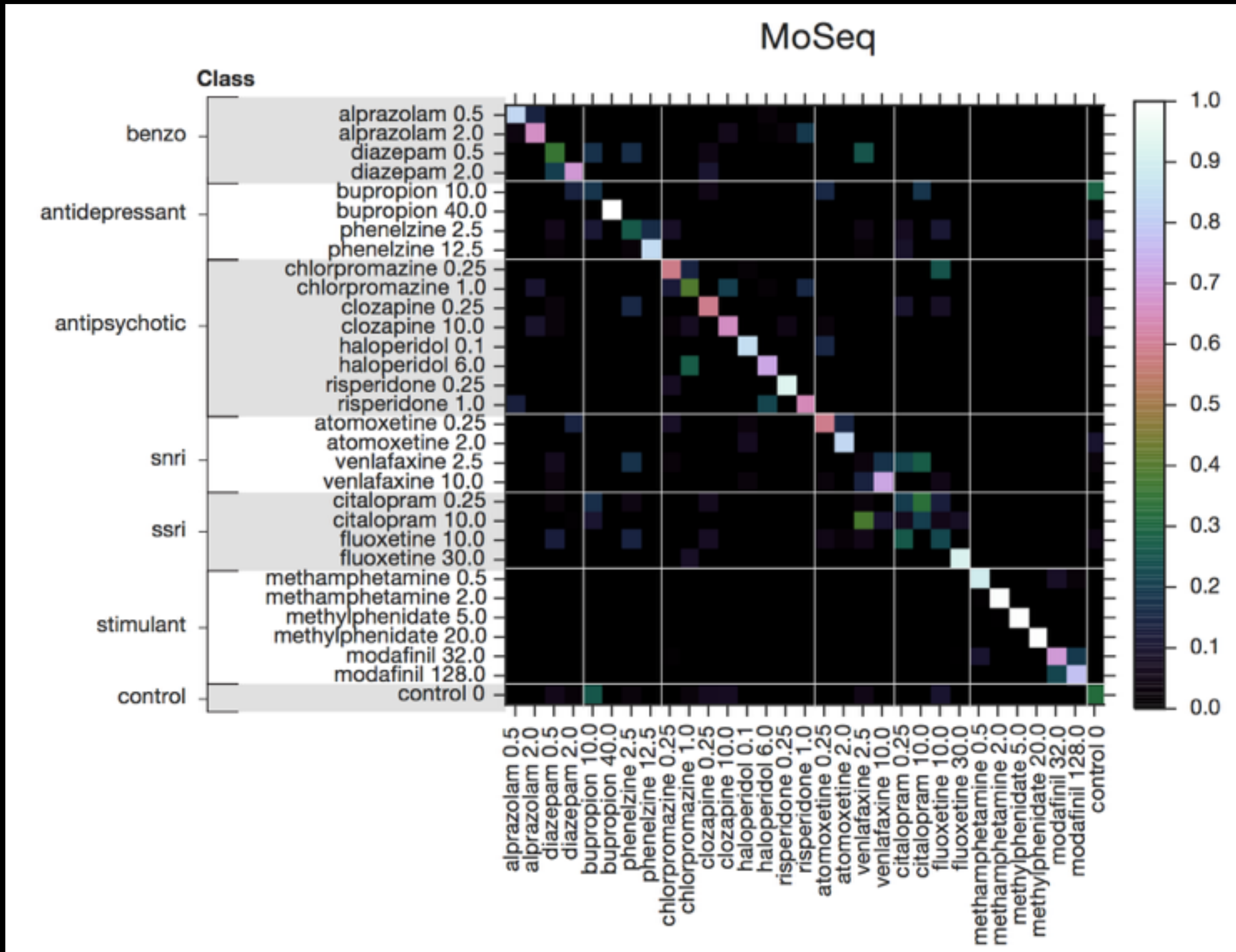
grooming

Discovery of Heterozygous Phenotypes in Ror1b Mice



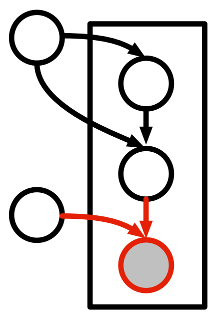
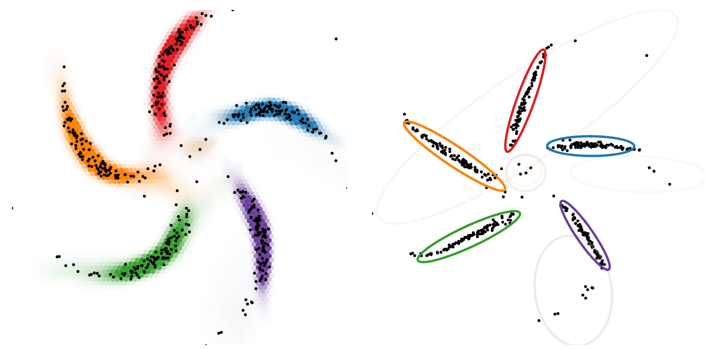
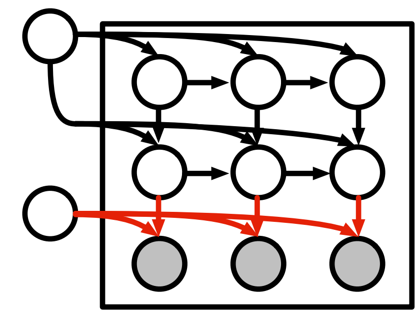
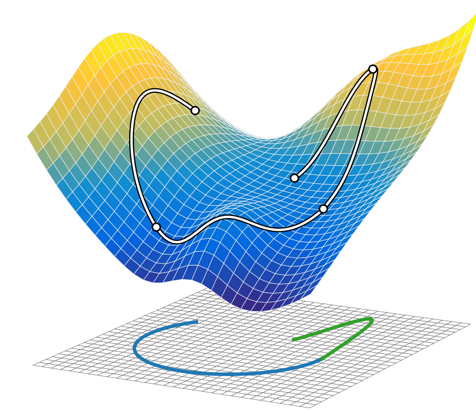
Alexander Wiltschko, **Matthew Johnson**, et al., Neuron 2015.

… and high and low doses of each drug

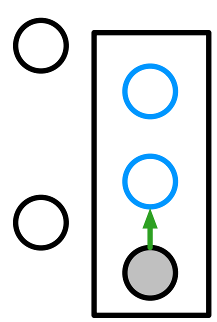
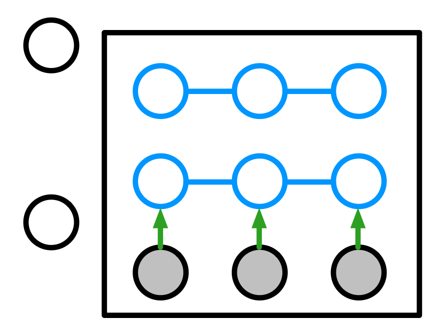


from Alex Wiltschko preprint

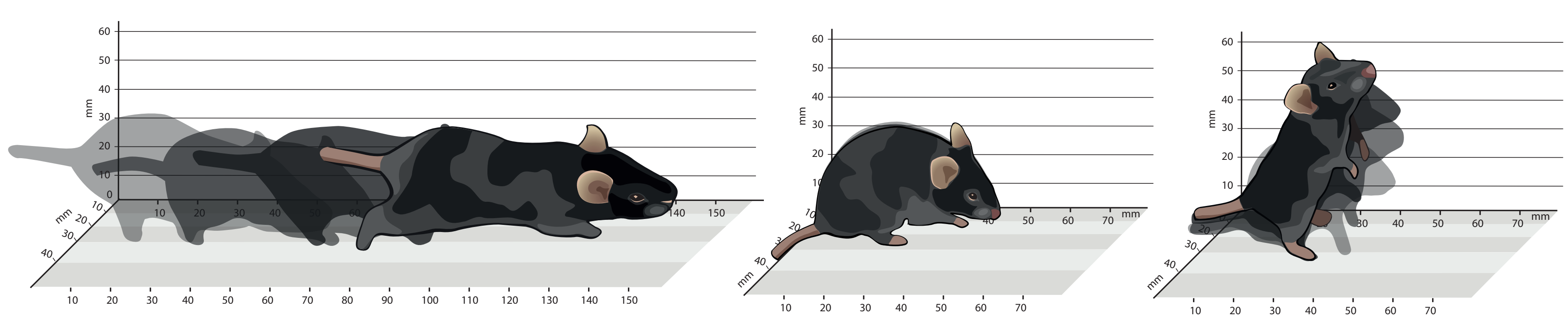
Modeling idea: graphical models on latent variables,
neural network models for observations

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

Application: learn syllable representation of behavior from video



Limitations and future work

capacity

- How expressive is latent linear structure?
  - word embeddings [1], analogical reasoning in image models
  - SVAE can use nonlinear latent structure

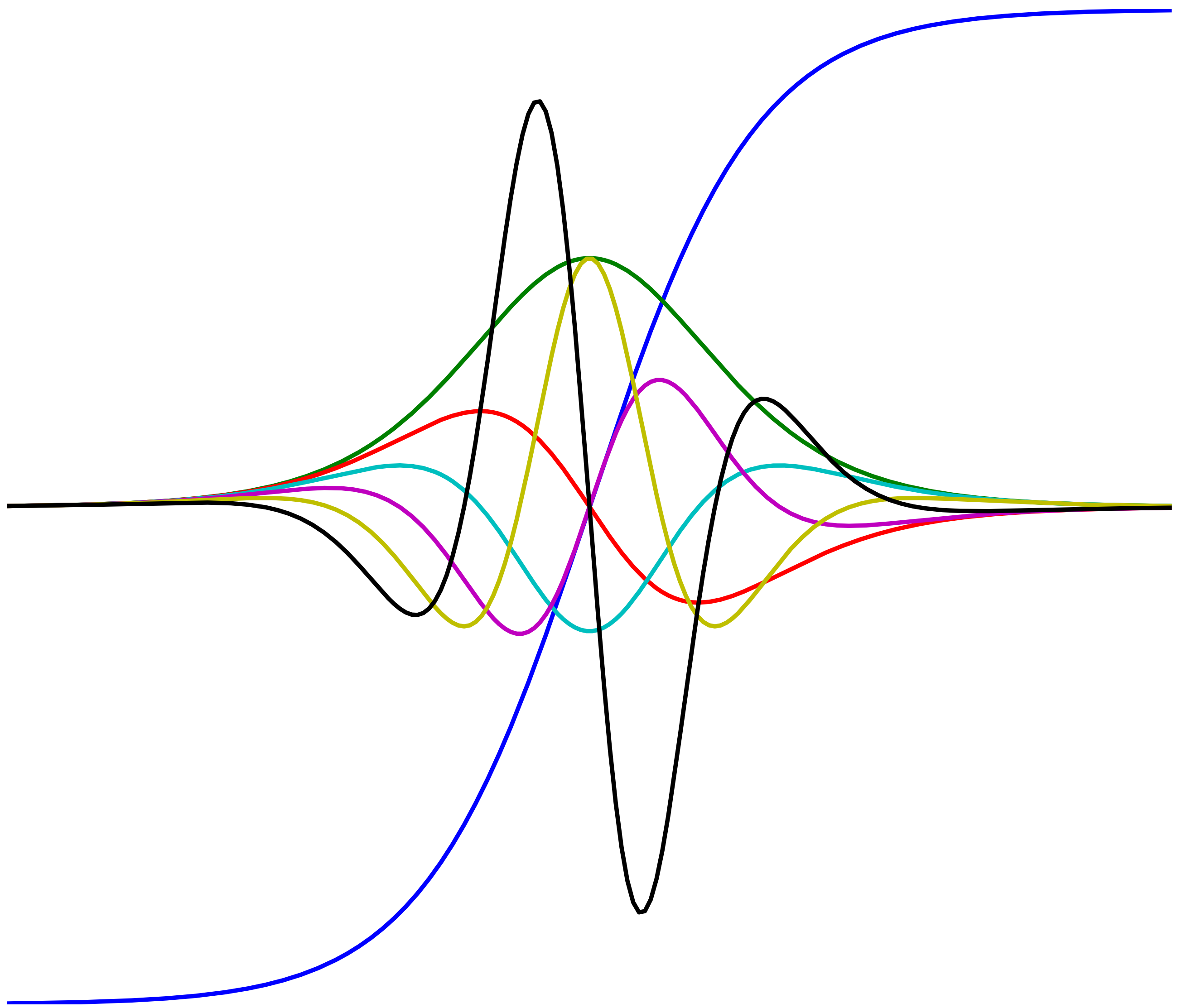
complexity

- PGMs get complicated
  - SVAE keeps complexity modular

future work

- model-based reinforcement learning
- automatic structure search [2,3]
- semi-supervised applications

[1] Hashimoto, Alvarez-Melis, and Jaakkola, Word, graph and manifold embedding from Markov processes, Preprint 2015.
[2] Grosse et al., Exploiting compositionality to explore a large space of model structures, UAI 2012.
[3] Duvenaud et al., Structure discovery in nonparametric regression through compositional kernel search, ICML 2013.



github.com/hips/autograd

Thanks!