Deep Unsupervised Learning using Nonequilibrium Thermodynamics

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Outline

- Motivation: The promise of deep unsupervised learning
- Physical intuition: Diffusion processes and time reversal
- Diffusion probabilistic model: Derivation and experimental results
- Other projects: Training energy based models, Monte Carlo, deep learning theory

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- **Motivation: The promise of deep unsupervised learning**
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The Promise of Deep Unsupervised Learning

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  - Novel modalities

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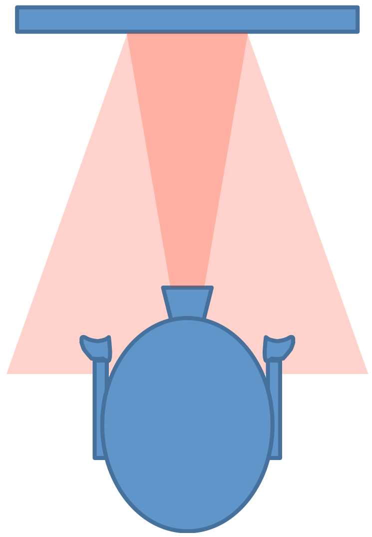

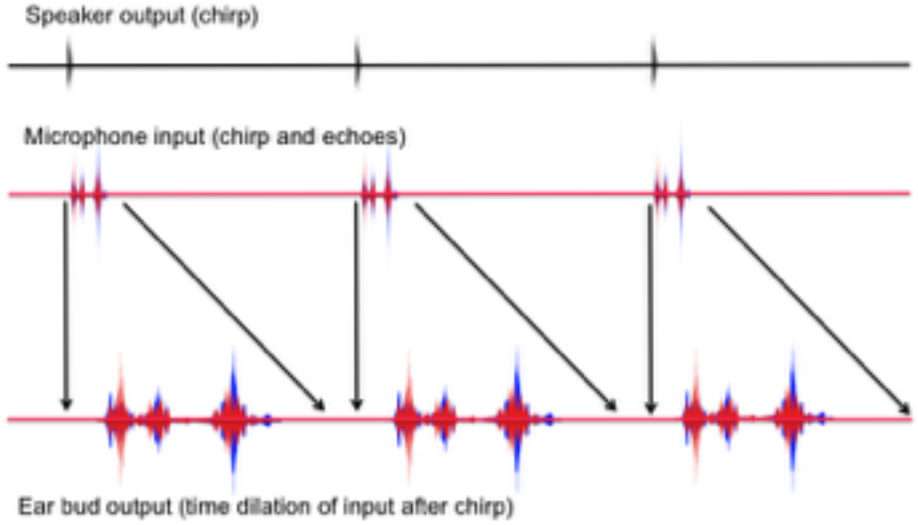

[Trans Biomed Eng, 2015]

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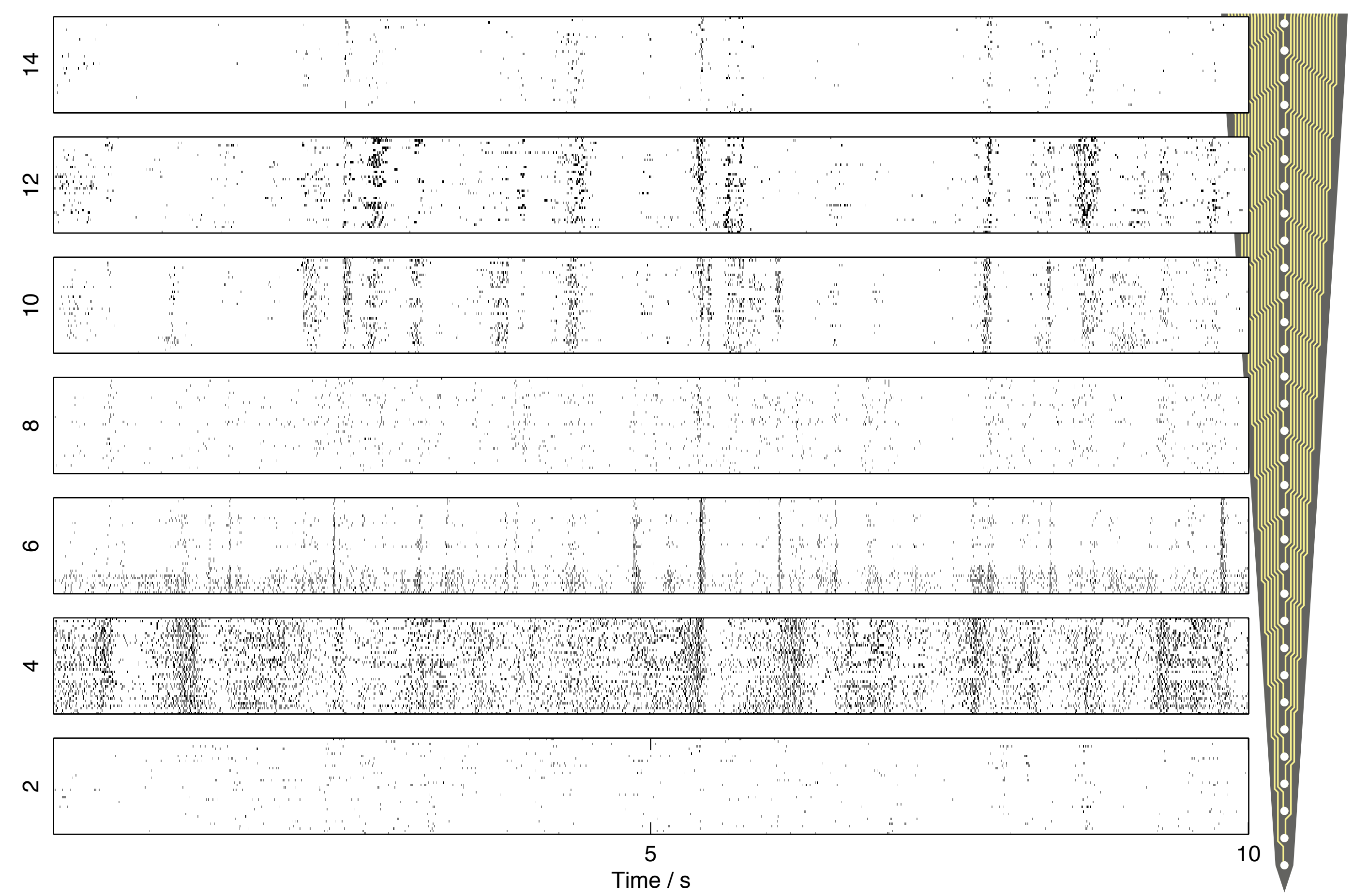
7 exemplar multiunits responding to 40 repeated trials of natural video in cat V1



[PLoS Comp Bio 2014] [Neuron 2013]

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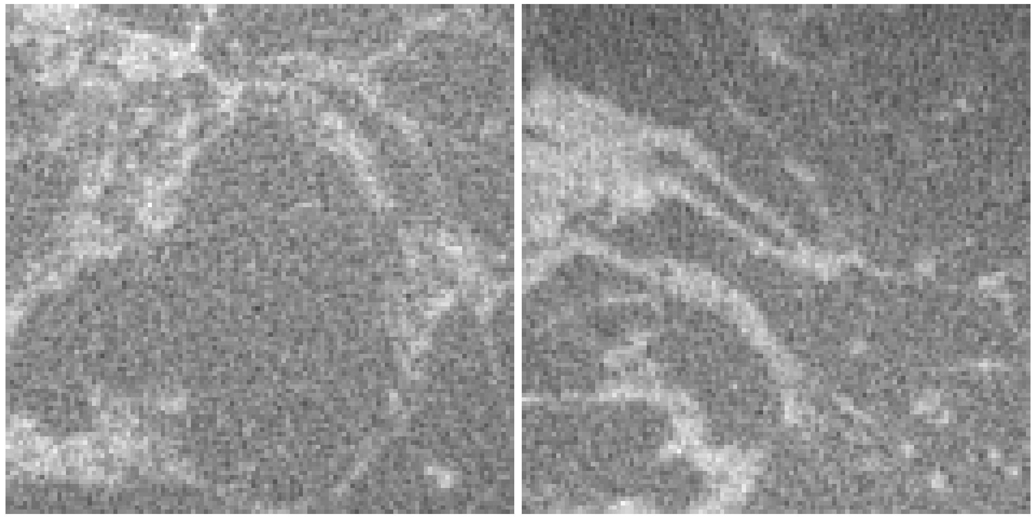
Coronal breast CT



[SPIE 2009] [Med Phys 2014]

The Promise of Deep Unsupervised Learning

- Unknown features/labels
  - Novel modalities
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The Promise of Deep Unsupervised Learning

- Unknown features/labels
  - Novel modalities
  - Exploratory data analysis
- Expensive labels
- Unpredictable tasks / one shot learning

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- Motivation: The promise of deep unsupervised learning
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- Diffusion probabilistic model: Derivation and experimental results
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Outline

- Motivation: The promise of deep unsupervised learning
- **Physical intuition: Diffusion processes and time reversal**
    - Destroy structure in data
    - Carefully characterize the destruction
    - Learn how to **reverse time**
- Diffusion probabilistic model: Derivation and experimental results
- Other projects: Training energy based models, Monte Carlo, deep learning theory

Observation 1: Diffusion Destroys Structure

- Dye density represents probability density

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Data distribution → Uniform distribution

Core Idea: Recover Structure by Reversing Time

- What if we could reverse time?

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- What if we could reverse time?

Data distribution ← Uniform distribution

Core Idea: Recover Structure by Reversing Time

- What if we could reverse time?
- Recover data distribution by starting from uniform distribution and running dynamics backwards

Data distribution ← Uniform distribution

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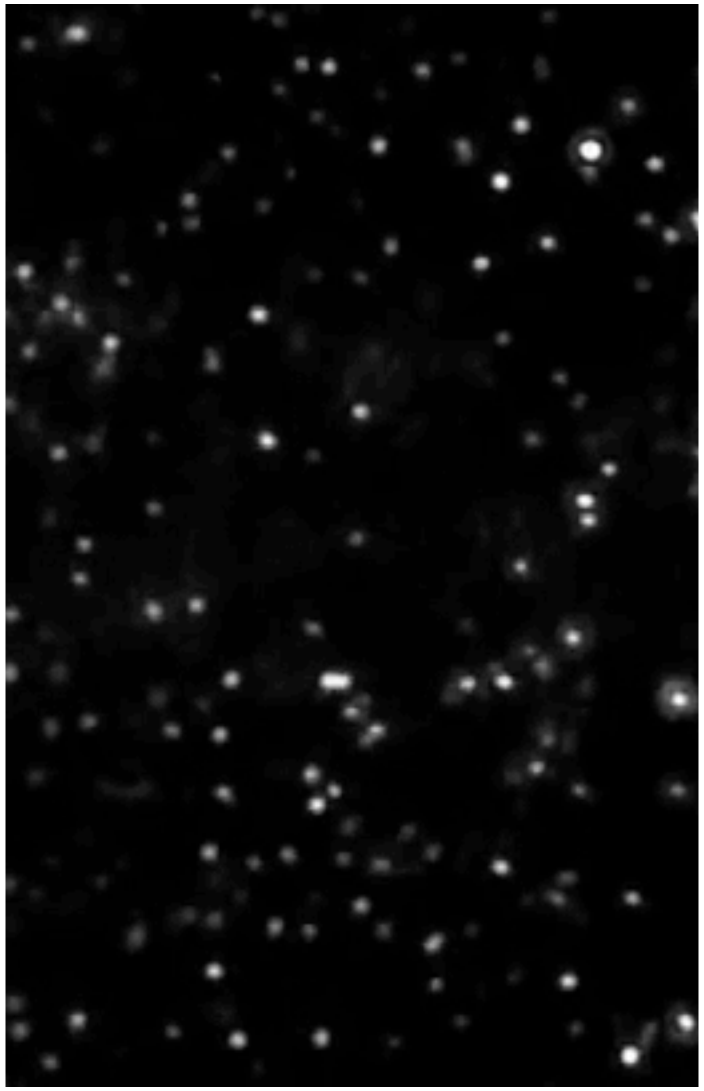
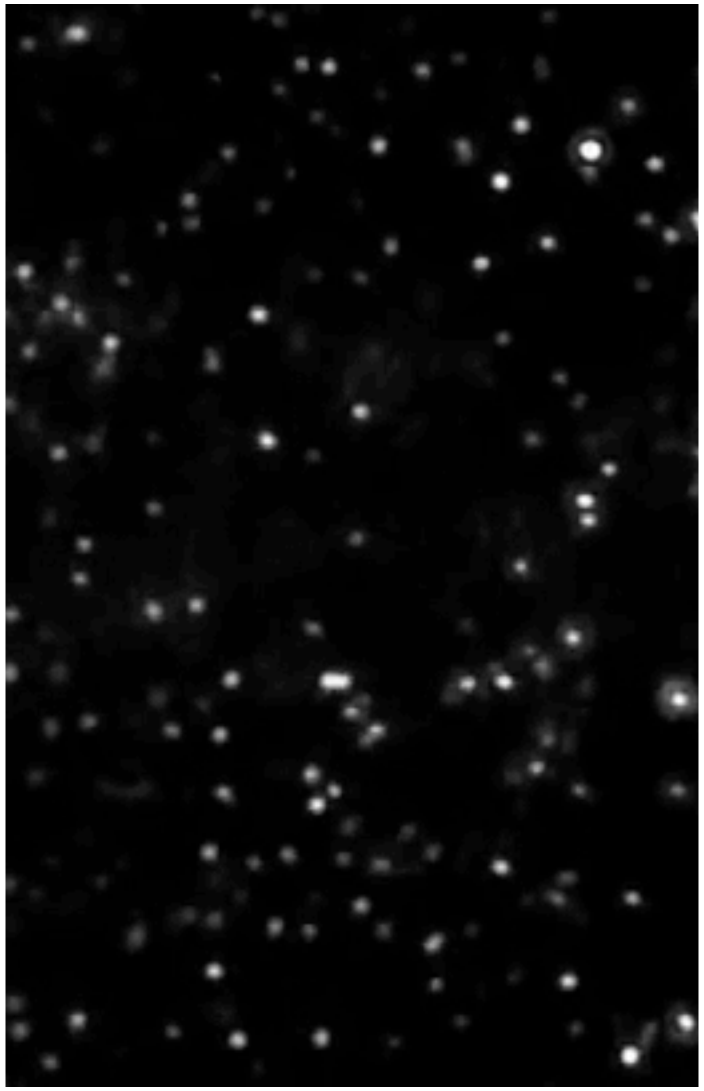
Observation 2: Microscopic Diffusion is Time Reversible



- Microscopic view
- Brownian motion

Observation 2: Microscopic Diffusion is Time Reversible



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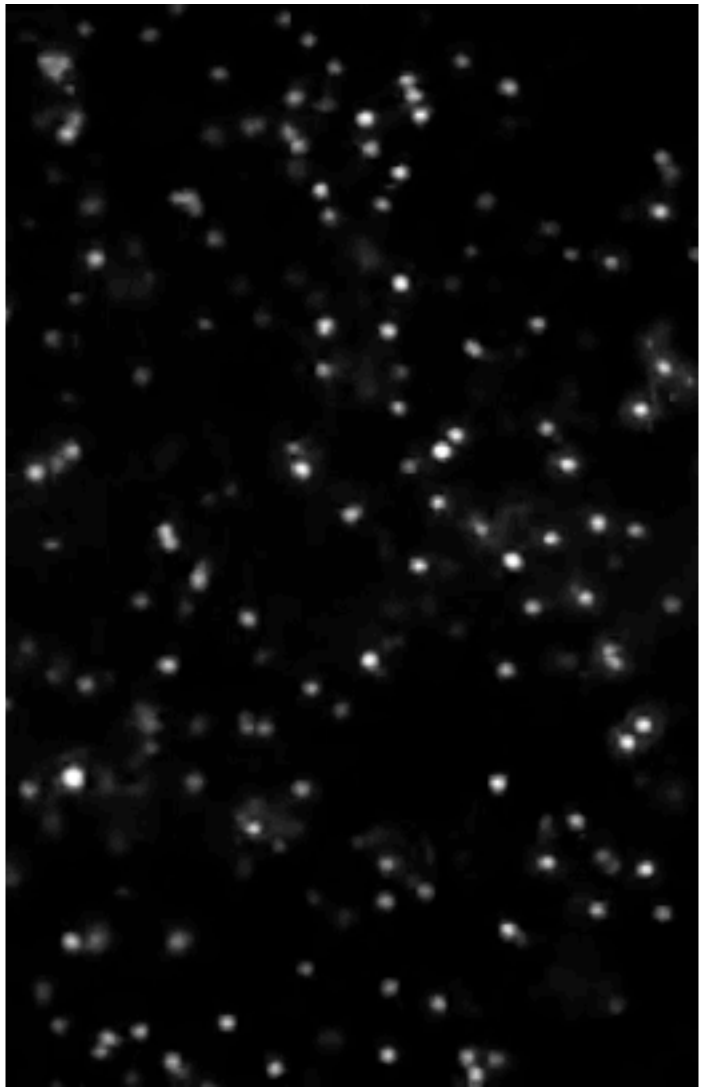

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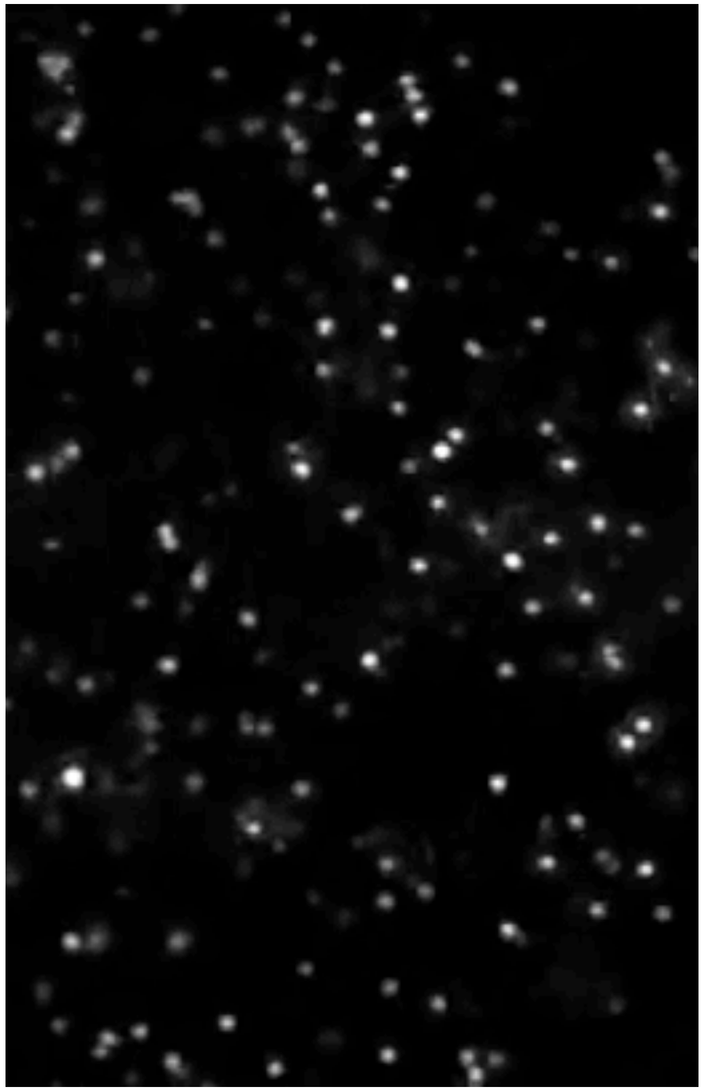

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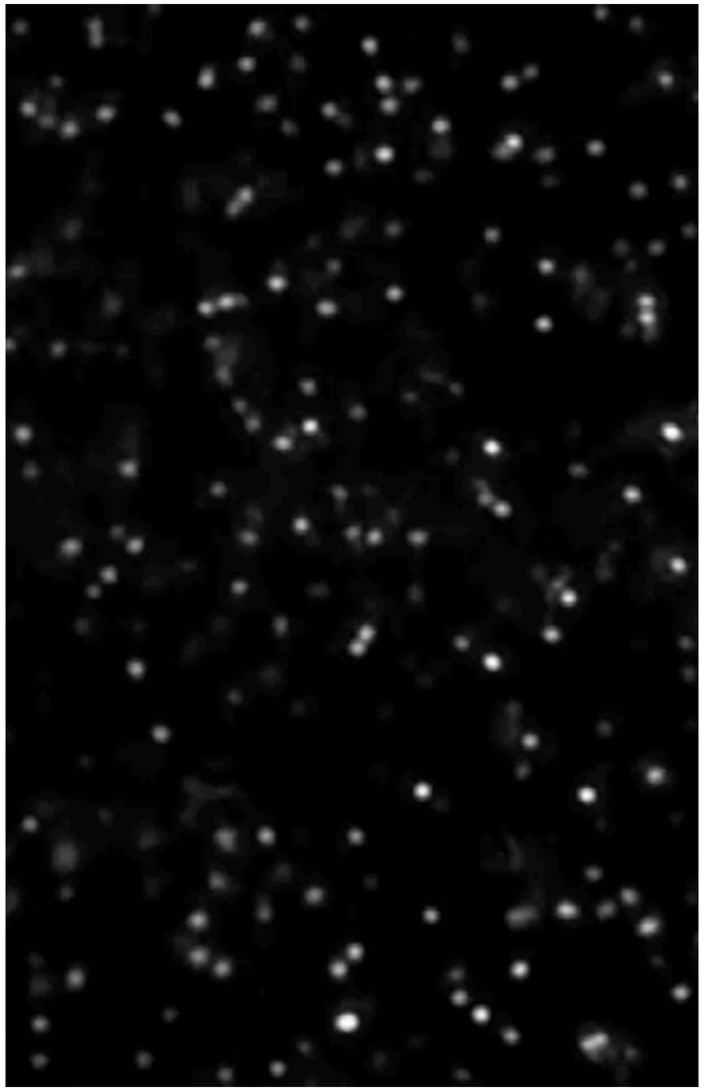

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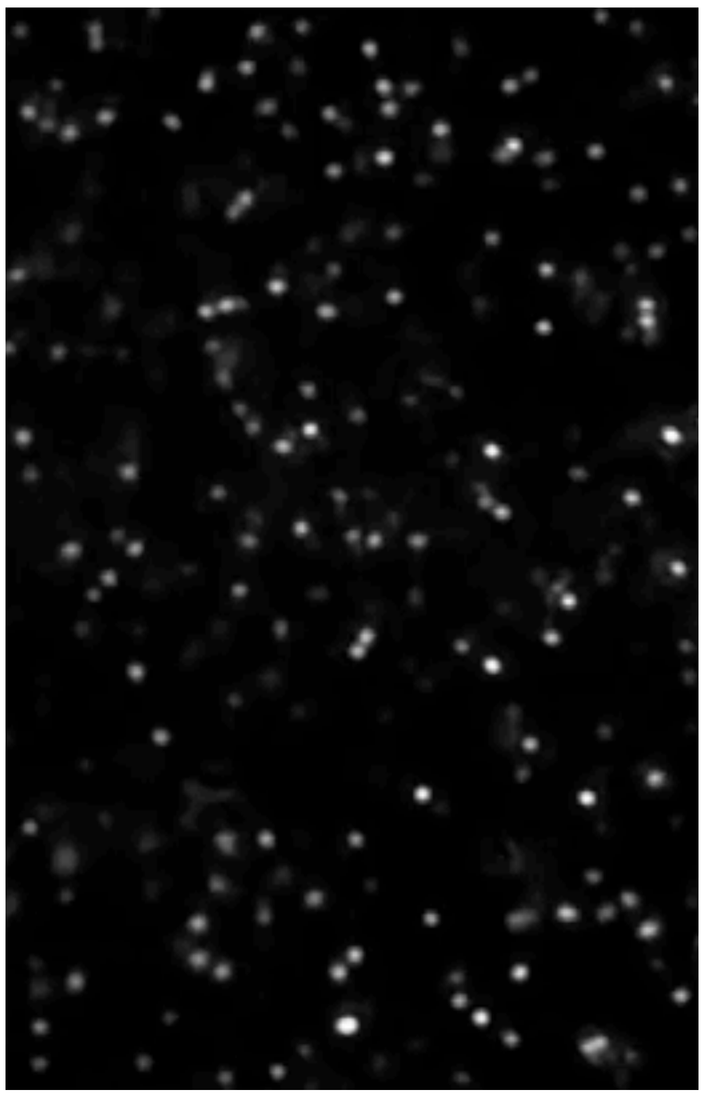

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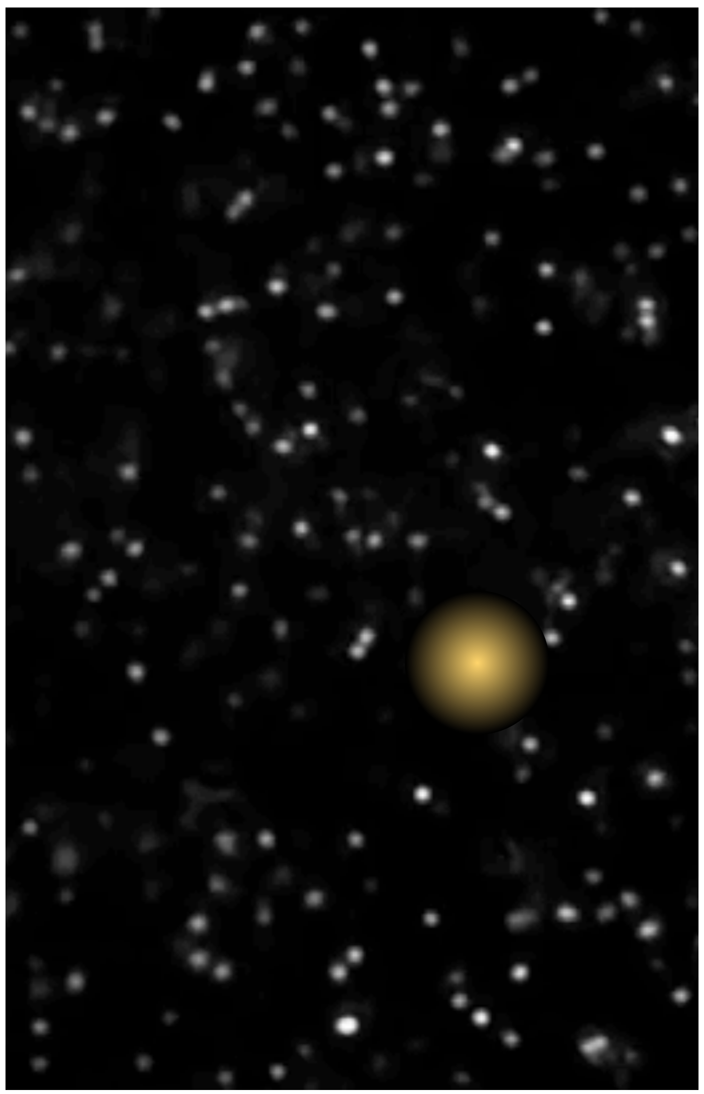

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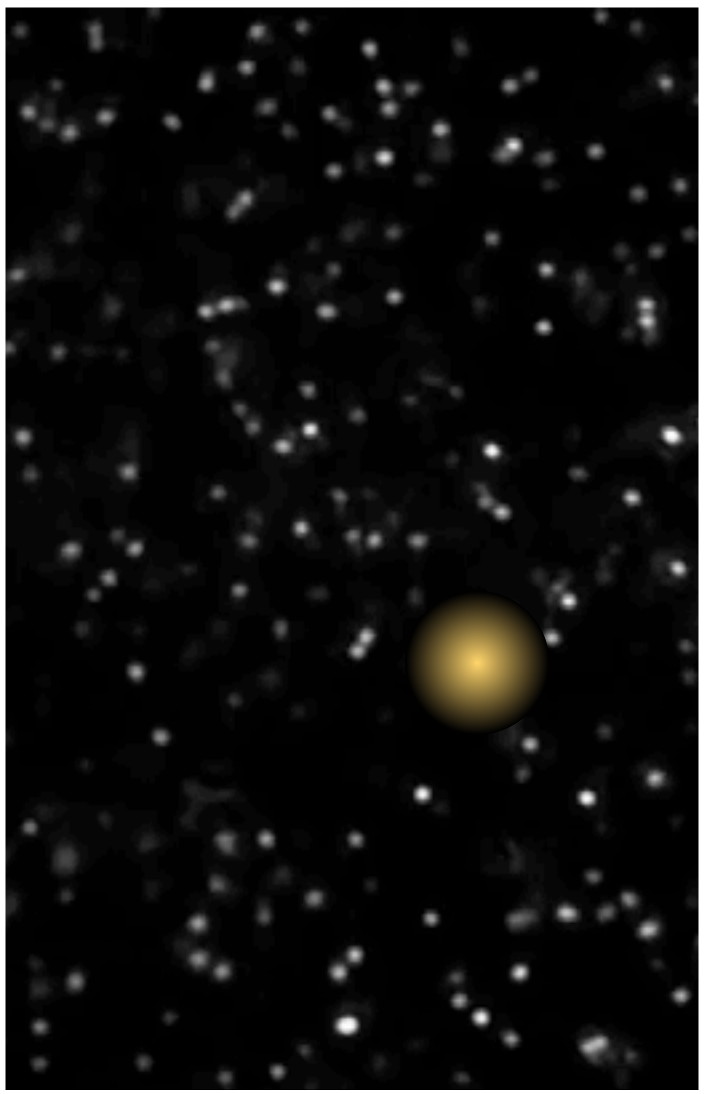
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- Microscopic view
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- Position updates are small Gaussians
    - Both forwards and backwards in time

Overview of Diffusion-based Probabilistic Models

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- Destroy all structure in data distribution using diffusion process

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- Destroy all structure in data distribution using diffusion process
- Learn reversal of diffusion process
    - Estimate function for mean and covariance of each step in the reverse diffusion process (binomial rate for binary data)
- Reverse diffusion process is the model of the data

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  - Deep convolutional network: Universal function approximator
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Destroy All Structure in Data using Diffusion Process

Data distribution

$$q\left(\mathbf{x}^{(0)}\right)$$

Destroy All Structure in Data using Diffusion Process

Data distribution

Forward diffusion

$$q\left(\mathbf{x}^{(0)}\right)$$

$$q\left(\mathbf{x}^{(t)}|\mathbf{x}^{(t-1)}\right) = \mathcal{N}\left(\mathbf{x}^{(t)};\mathbf{x}^{(t-1)}\sqrt{1-\beta_t},\mathbf{I}\beta_t\right)$$

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Decay towards origin

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Decay towards origin

Add small noise

Destroy All Structure in Data using Diffusion Process

Data distribution	Forward diffusion	Noise distribution
$q\left(\mathbf{x}^{(0)}\right)$		$q\left(\mathbf{x}^{(T)}\right) \approx \mathcal{N}\left(\mathbf{x}^{(T)}; 0, \mathbf{I}\right)$

$$q\left(\mathbf{x}^{(t)} | \mathbf{x}^{(t-1)}\right) = \mathcal{N}\left(\mathbf{x}^{(t)}; \mathbf{x}^{(t-1)}\sqrt{1-\beta_t}, \mathbf{I}\beta_t\right)$$

Decay towards origin

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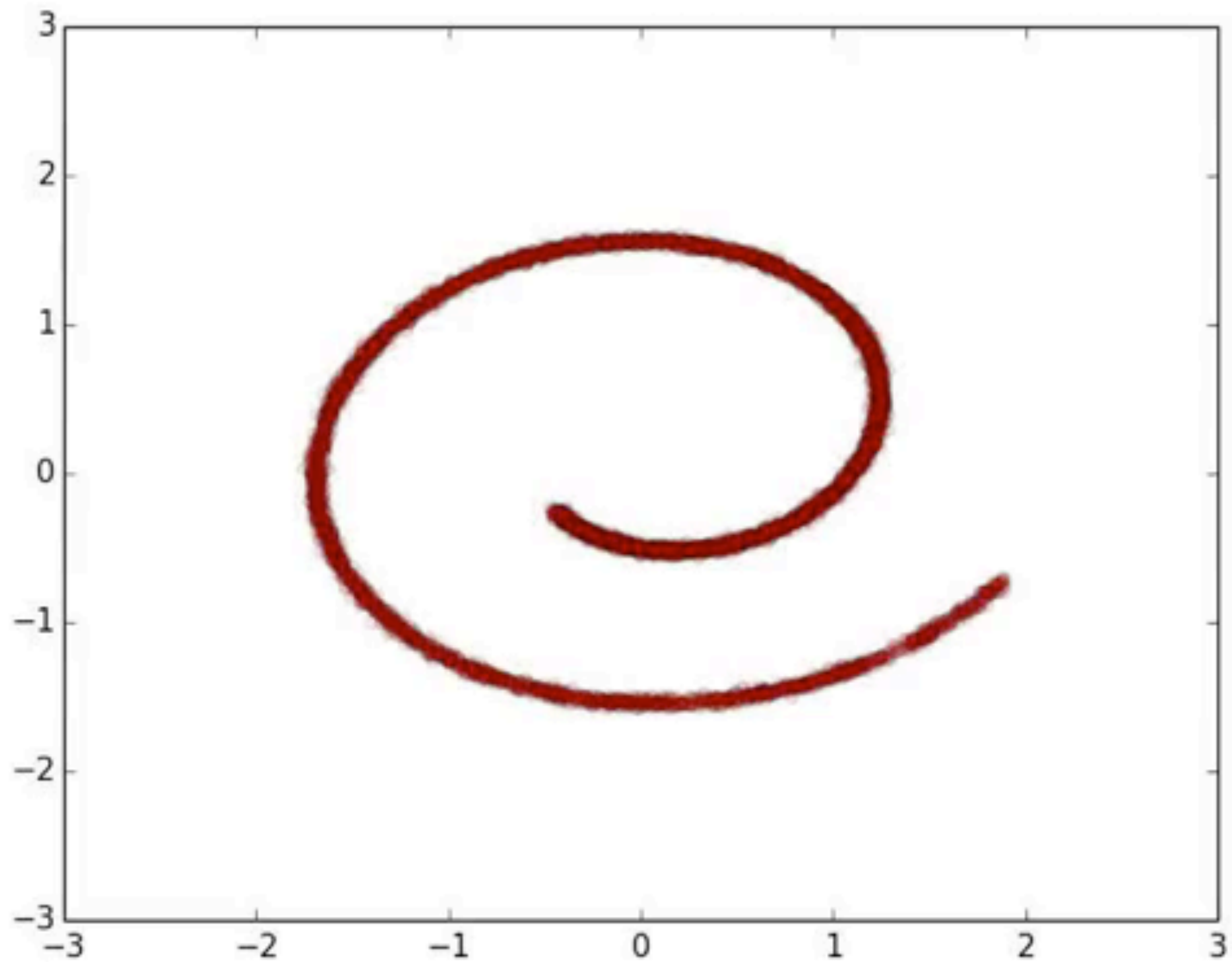
Forward Diffusion Process on Swiss Roll

- Start at data
- Run Gaussian diffusion until samples become Gaussian blob



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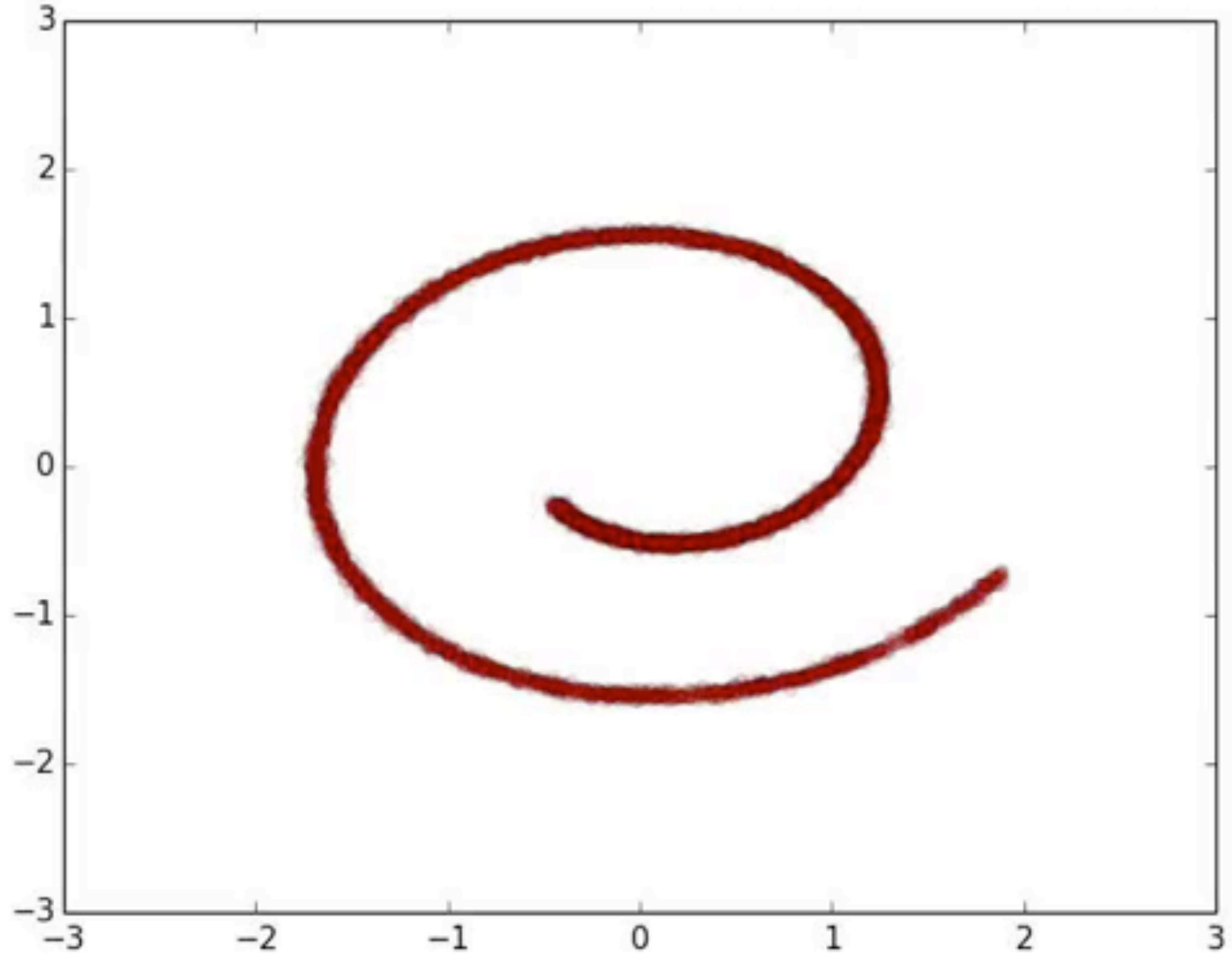

Recover Structure in Data using Reversal of Diffusion Process

Noise distribution

$$p\left(\mathbf{x}^{(T)}\right) = \mathcal{N}\left(\mathbf{x}^{(T)}; 0, \mathbf{I}\right)$$

Recover Structure in Data using Reversal of Diffusion Process

Reverse diffusion

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Learned drift and covariance functions

Recover Structure in Data using Reversal of Diffusion Process

Data distribution | Reverse diffusion | Noise distribution

$$p\left(\mathbf{x}^{(0)}\right) \approx q\left(\mathbf{x}^{(0)}\right) \longleftarrow p\left(\mathbf{x}^{(T)}\right) = \mathcal{N}\left(\mathbf{x}^{(T)}; 0, \mathbf{I}\right)$$

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Learned Reverse Diffusion Process on Swiss Roll

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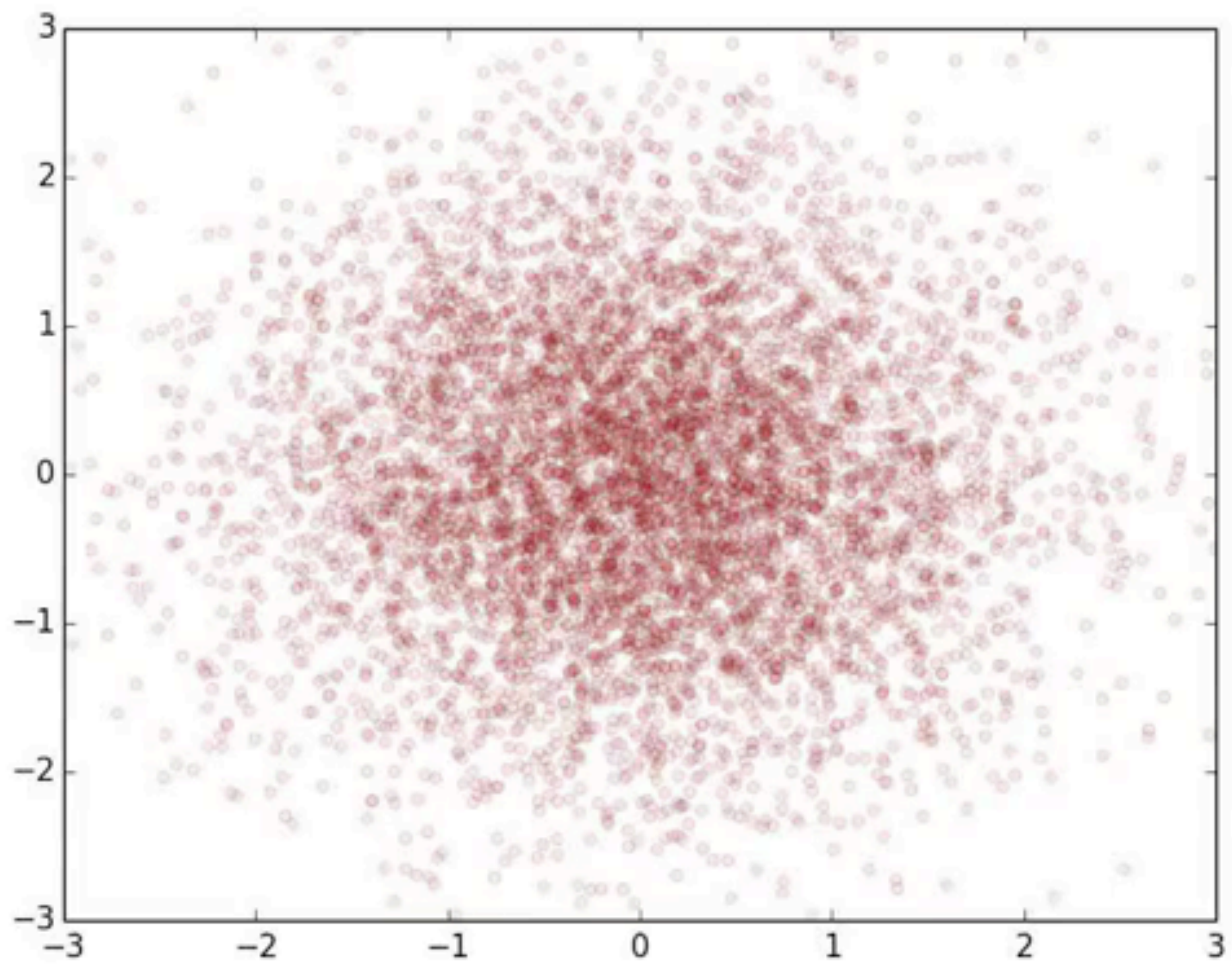

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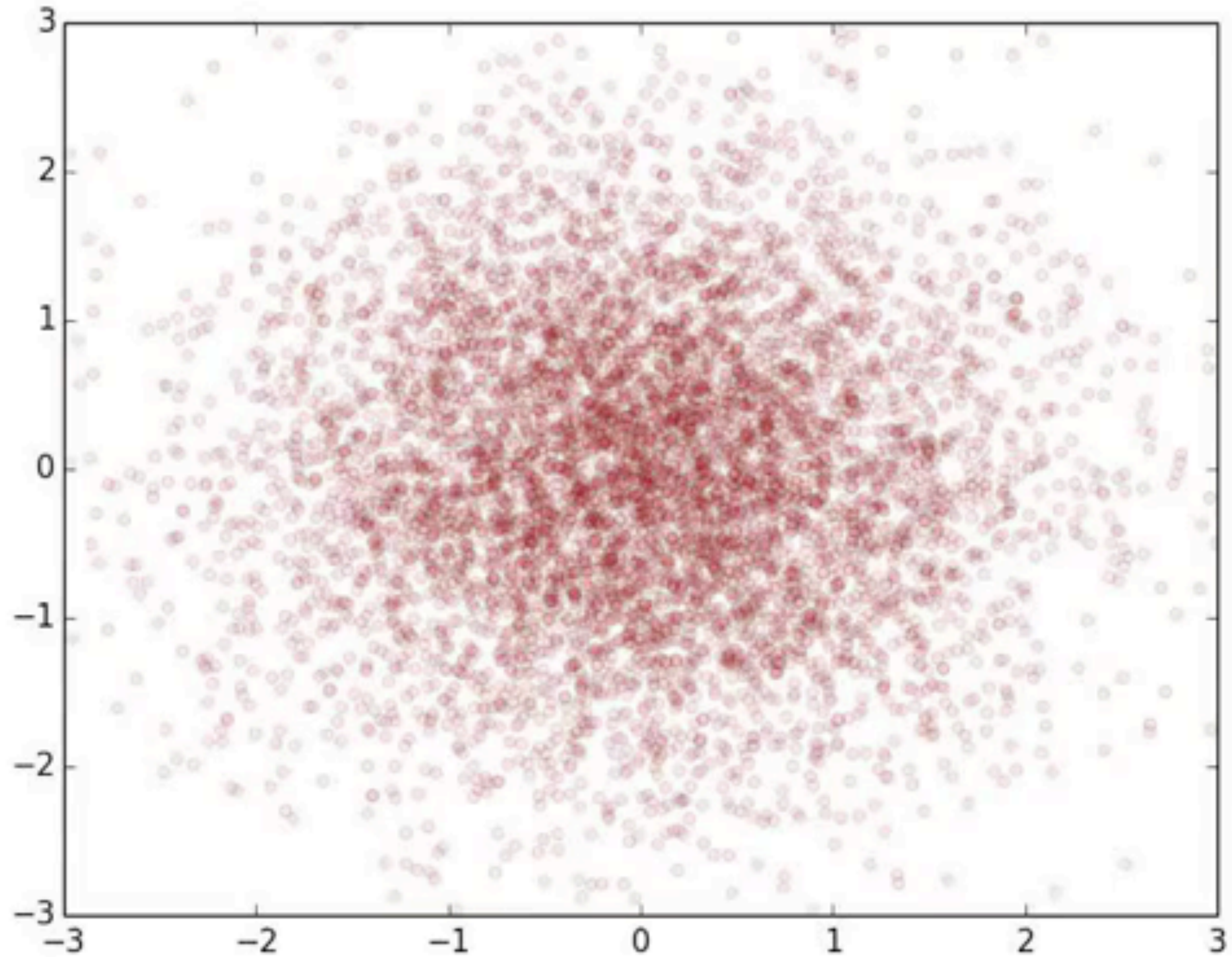
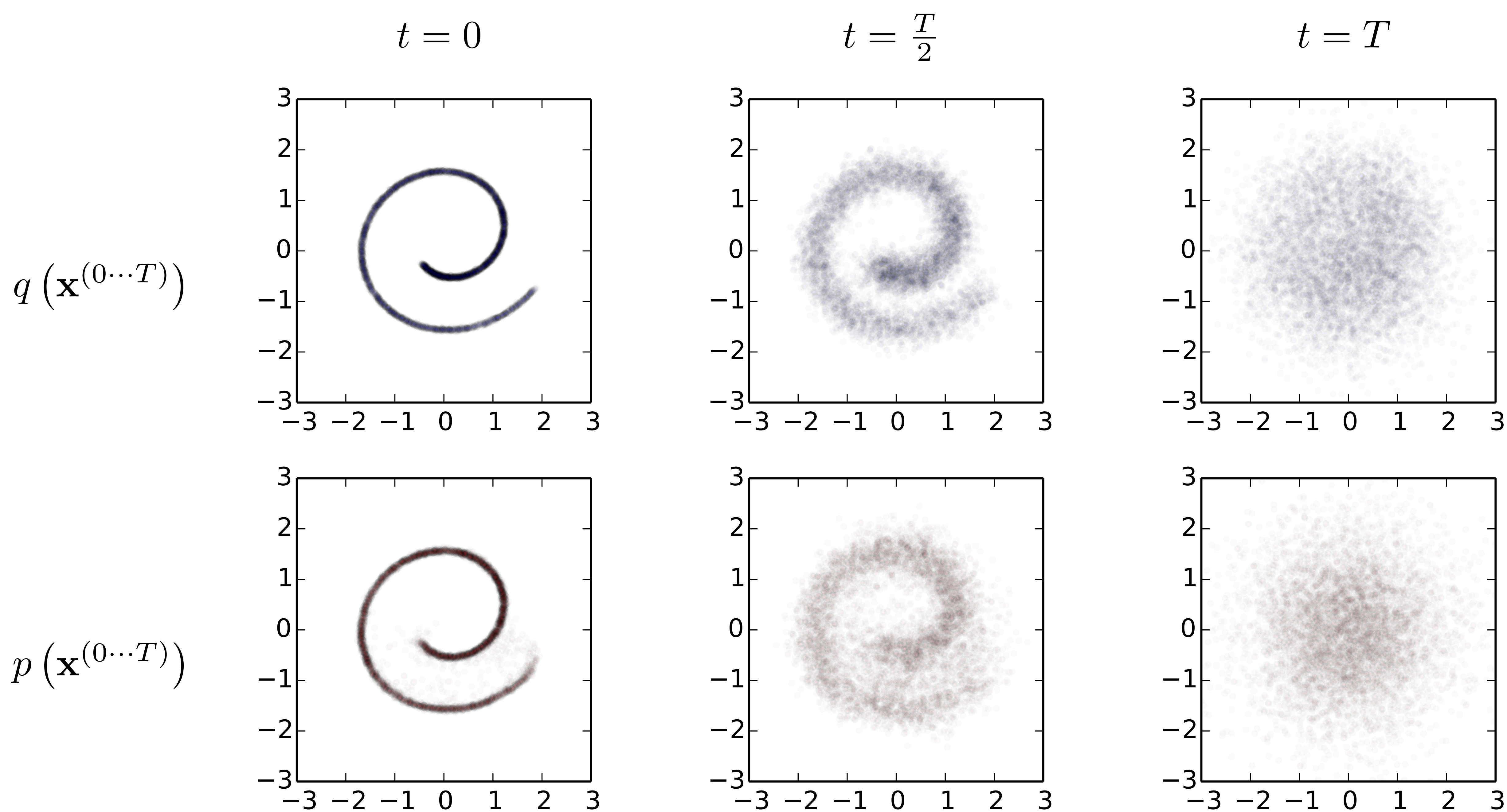


Summary of Forward and Reverse Diffusion on Swiss Roll



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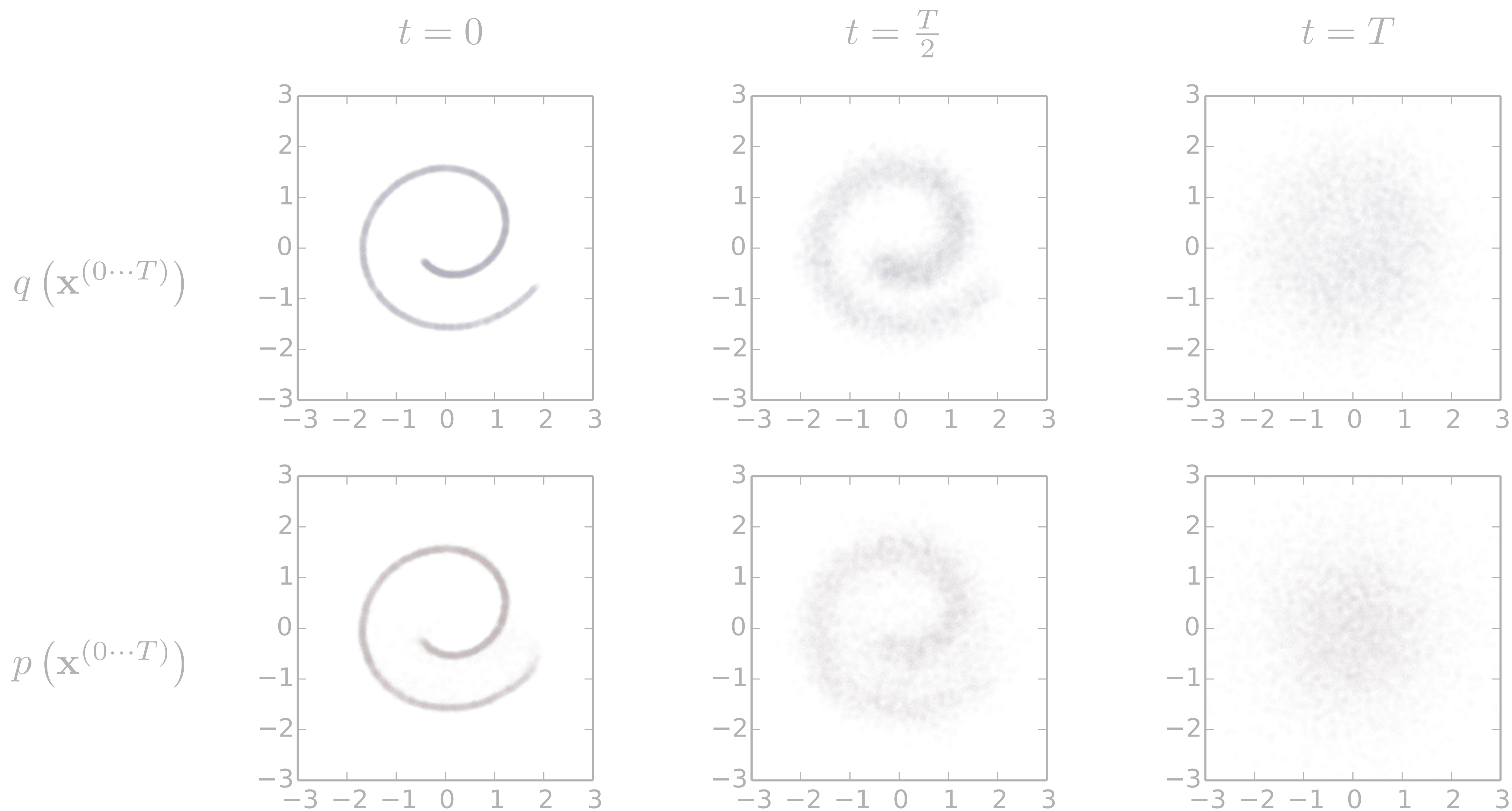

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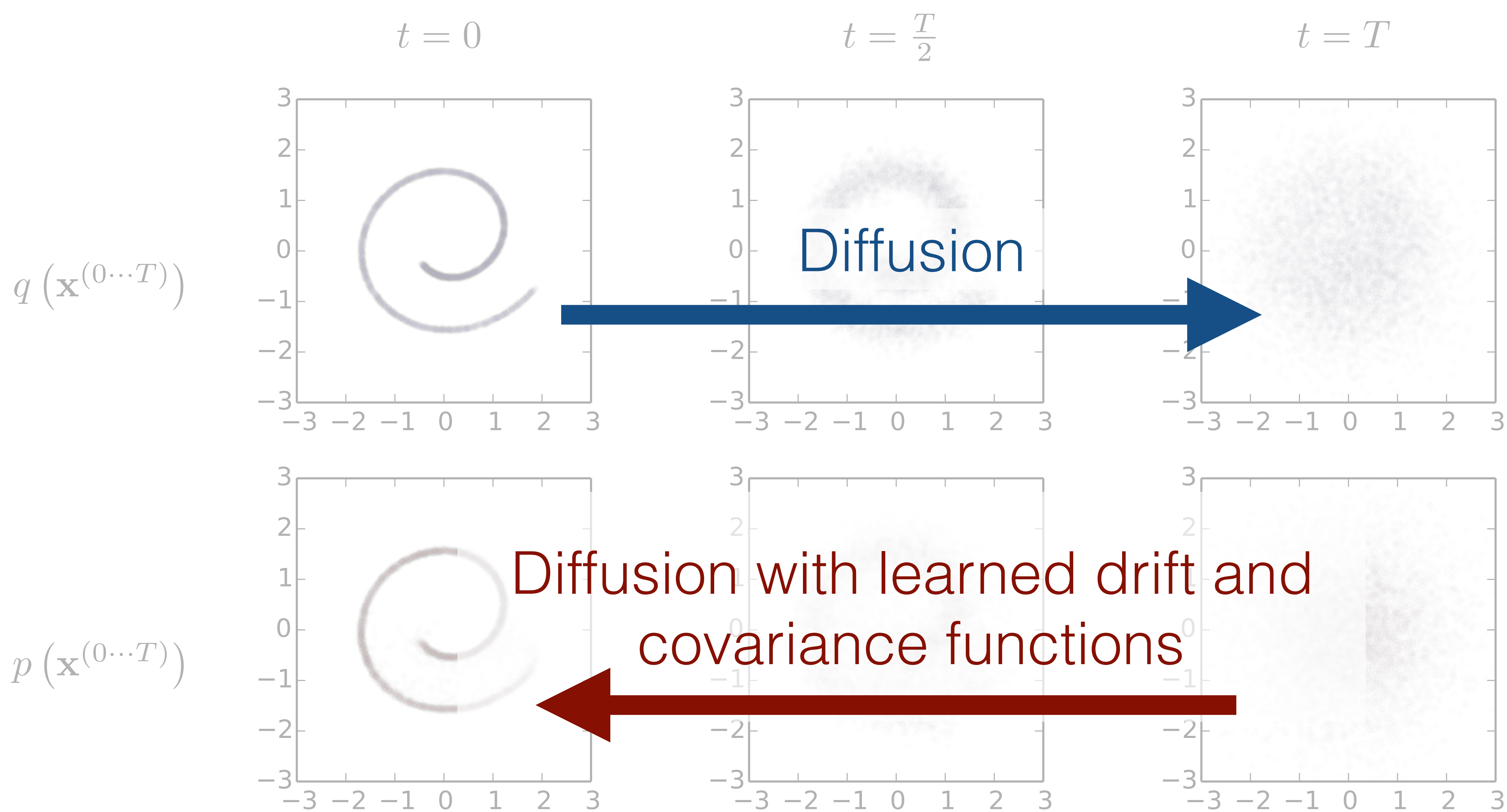

Training the Reverse Diffusion Process

Model probability

$$p\left(\mathbf{x}^{(0)}\right) = \int d\mathbf{x}^{(1\cdots T)} p\left(\mathbf{x}^{(0\cdots T)}\right)$$

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Annealed importance sampling / Jarzynski equality

$$p\left(\mathbf{x}^{(0)}\right) = \int d\mathbf{x}^{(1\cdots T)} q\left(\mathbf{x}^{(1\cdots T)} | \mathbf{x}^{(0)}\right) \frac{p\left(\mathbf{x}^{(0\cdots T)}\right)}{q\left(\mathbf{x}^{(1\cdots T)} | \mathbf{x}^{(0)}\right)}$$

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Log Likelihood

$$L = \int d\mathbf{x}^{(0)} q\left(\mathbf{x}^{(0)}\right) \log\left[\int d\mathbf{x}^{(1\cdots T)} q\left(\mathbf{x}^{(1\cdots T)}\right) \frac{p\left(\mathbf{x}^{(0\cdots T)}\right)}{q\left(\mathbf{x}^{(1\cdots T)}\right)}\right]$$

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Jensen's inequality

$$L \geq \int d\mathbf{x}^{(0\cdots T)} q\left(\mathbf{x}^{(0\cdots T)}\right) \log\left[\frac{p\left(\mathbf{x}^{(0\cdots T)}\right)}{q\left(\mathbf{x}^{(1\cdots T)}|\mathbf{x}^{(0)}\right)}\right]$$

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… algebra …

$$L \geq -\sum_{t=2}^{T} \int d\mathbf{x}^{(0)} d\mathbf{x}^{(t)} q\left(\mathbf{x}^{(0)}, \mathbf{x}^{(t)}\right) D_{KL}\left(q\left(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}, \mathbf{x}^{(0)}\right) \middle|\middle| p\left(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}\right)\right)$$

$$+ \text{const}$$

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Gaussian

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Gaussian

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Training

$$\underset{f_\mu\left(\mathbf{x}^{(t)}, t\right), f_\Sigma\left(\mathbf{x}^{(t)}, t\right)}{\operatorname{argmin}} \mathbb{E}\left[D_{KL}\left(q\left(\mathbf{x}^{(t-1)} | \mathbf{x}^{(t)}, \mathbf{x}^{(0)}\right) \middle|\middle| p\left(\mathbf{x}^{(t-1)} | \mathbf{x}^{(t)}\right)\right)\right]$$

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Unsupervised learning → Regression

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- Diffusion probabilistic model: Derivation and experimental results
  - Algorithm
  - **Deep convolutional network: Universal function approximator**
  - Multiplying distributions: Inputation, denoising, computing posteriors
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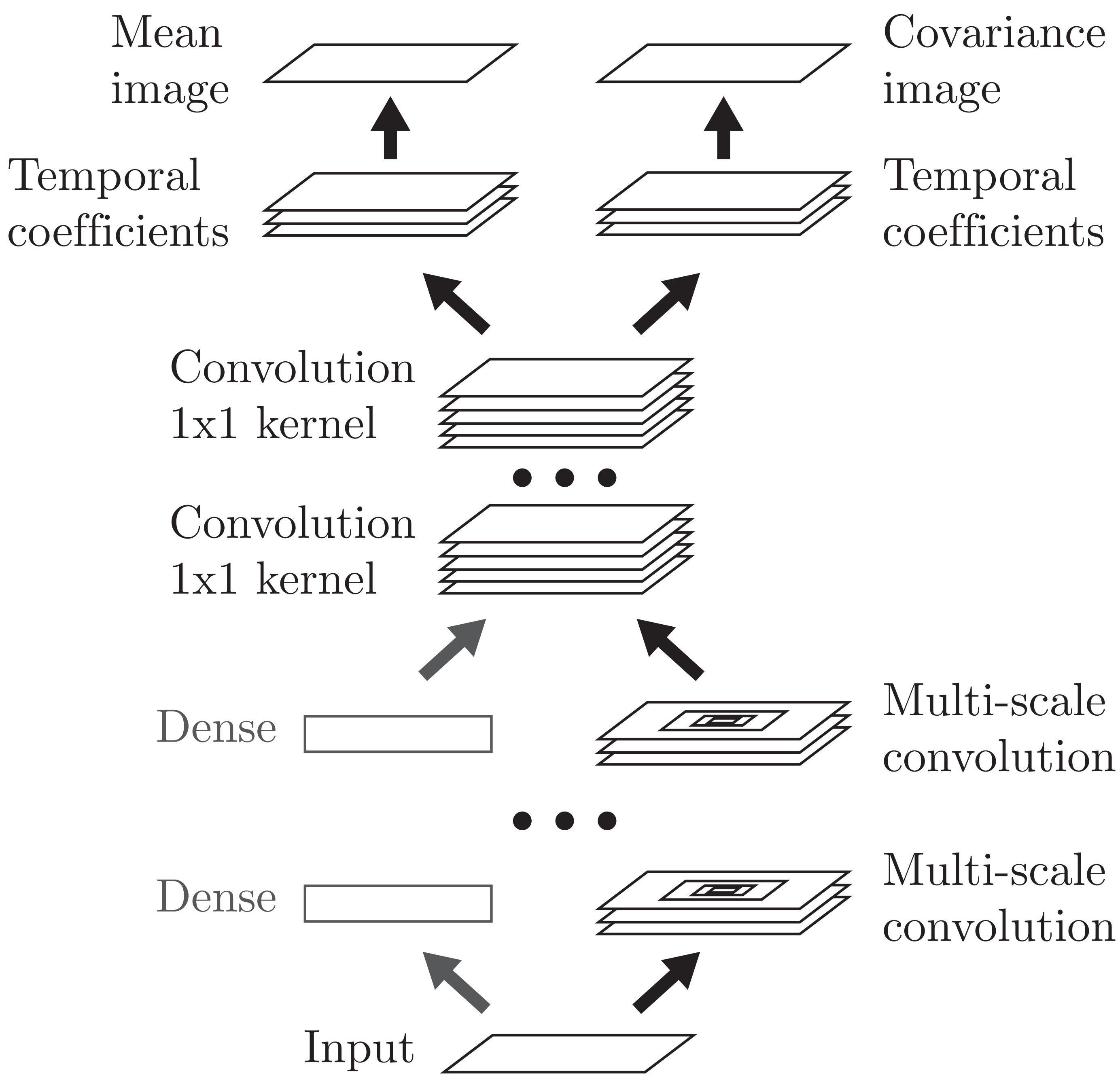
Use Deep Network as Function Approximator for Images



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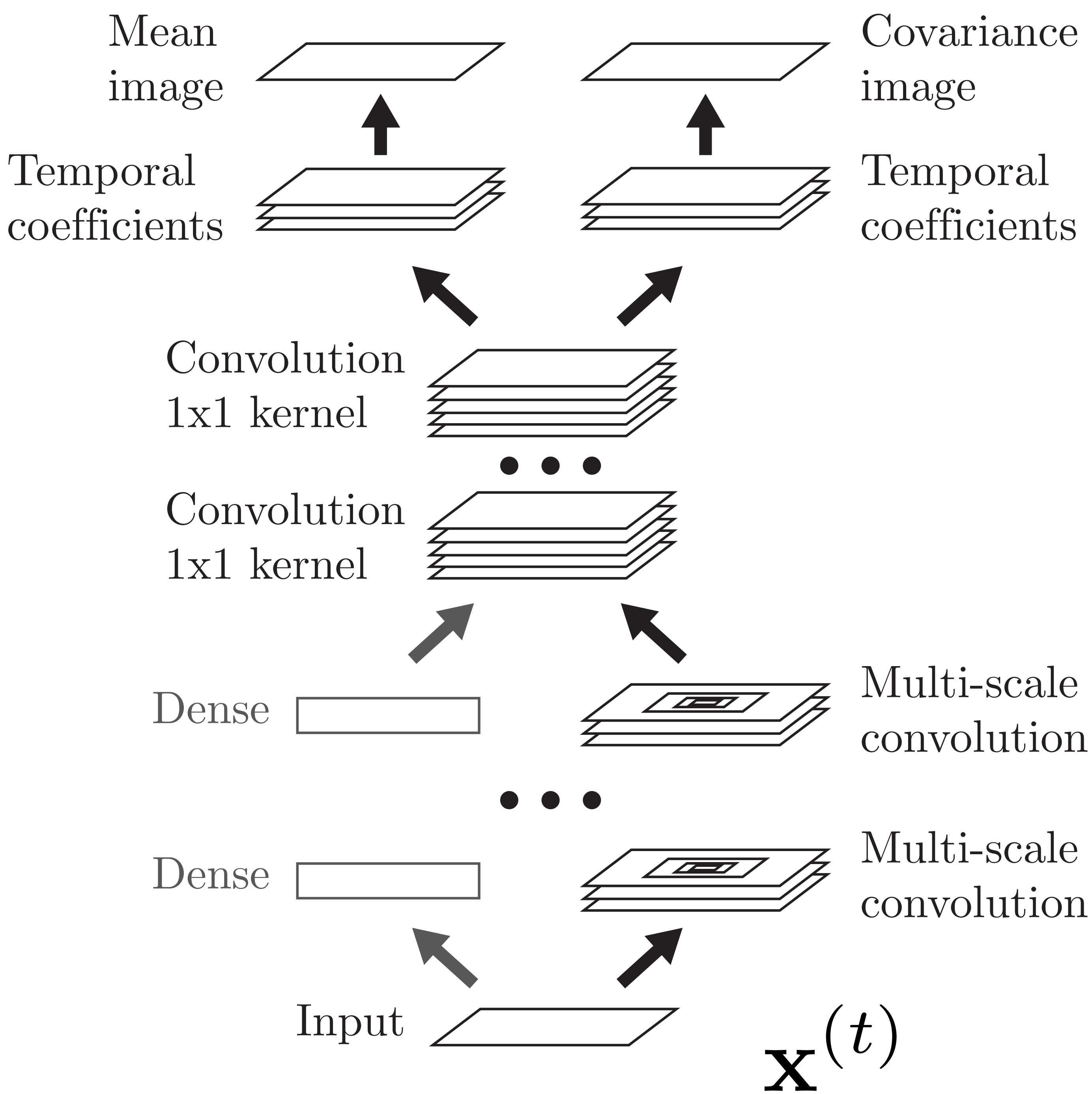
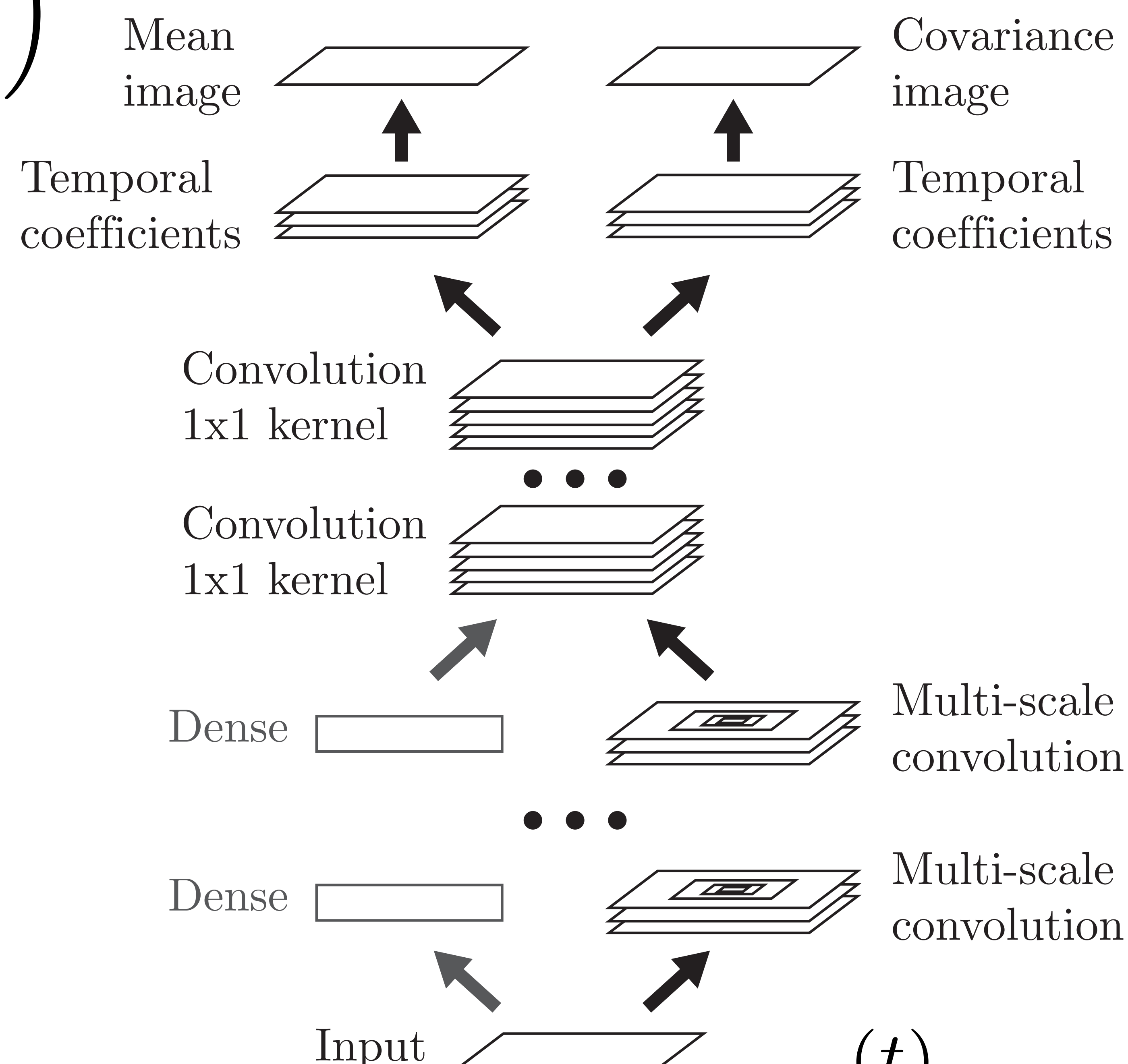


Use Deep Network as Function Approximator for Images

$f_\mu\left(\mathbf{x}^{(t)}, t\right)$

$f_\Sigma\left(\mathbf{x}^{(t)}, t\right)$



$\mathbf{x}^{(t)}$

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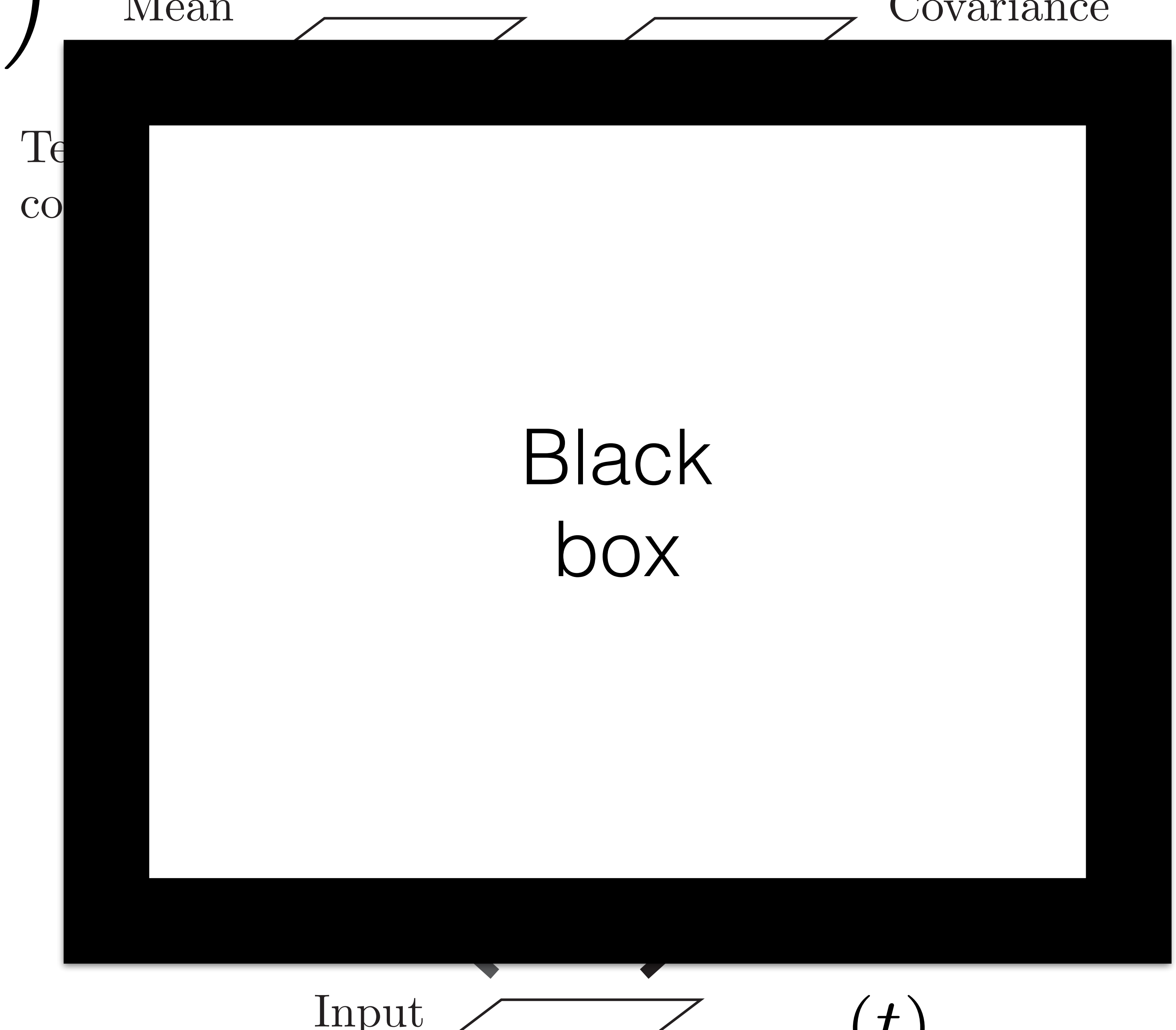
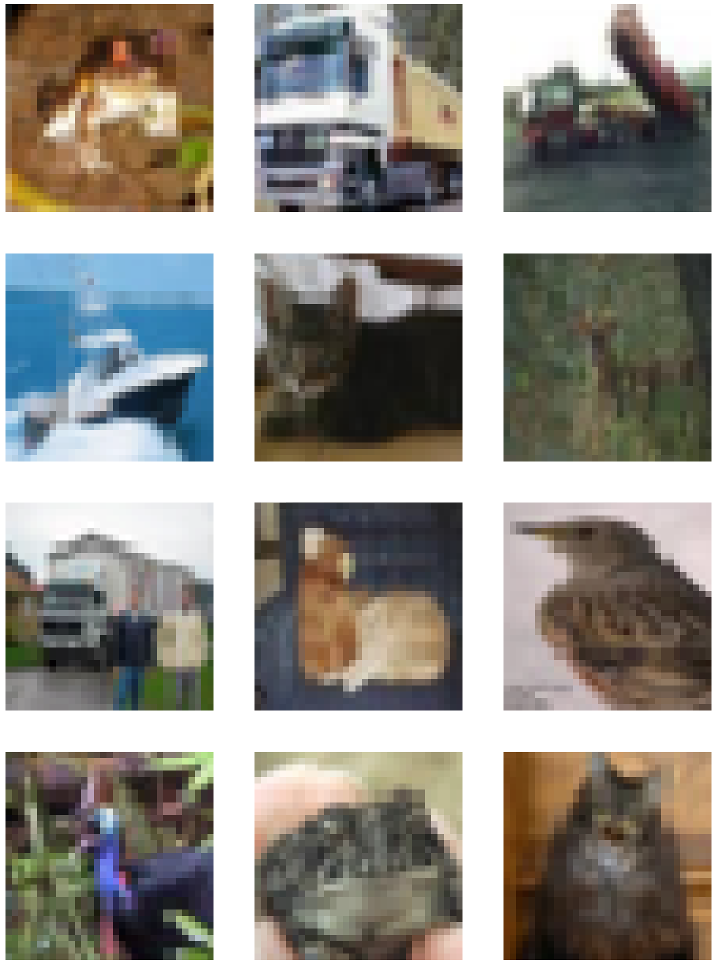
$$f_\Sigma\left(\mathbf{x}^{(t)}, t\right)$$



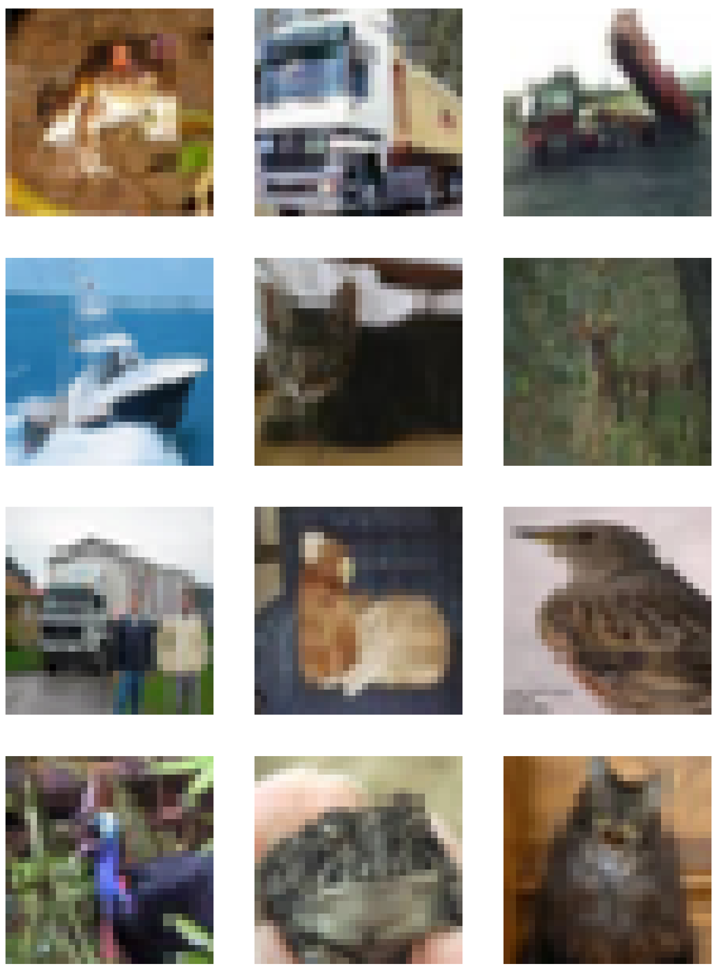
$$\mathbf{x}^{(t)}$$

Diffusion Probabilistic Model Applied to CIFAR-10



Training Data

Diffusion Probabilistic Model Applied to CIFAR-10



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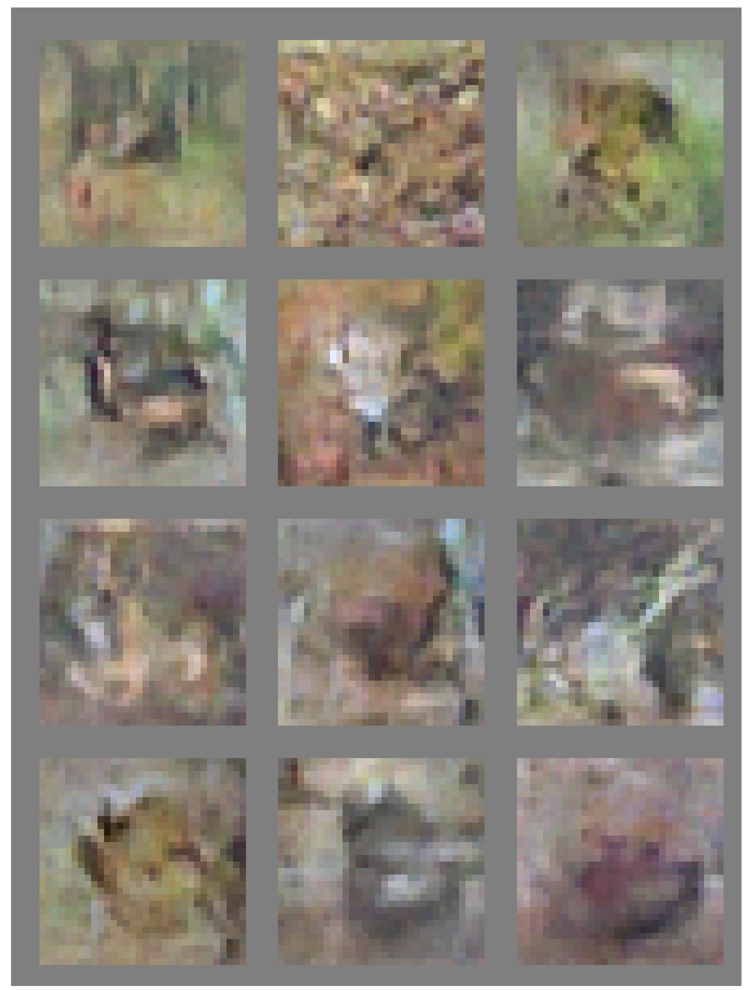
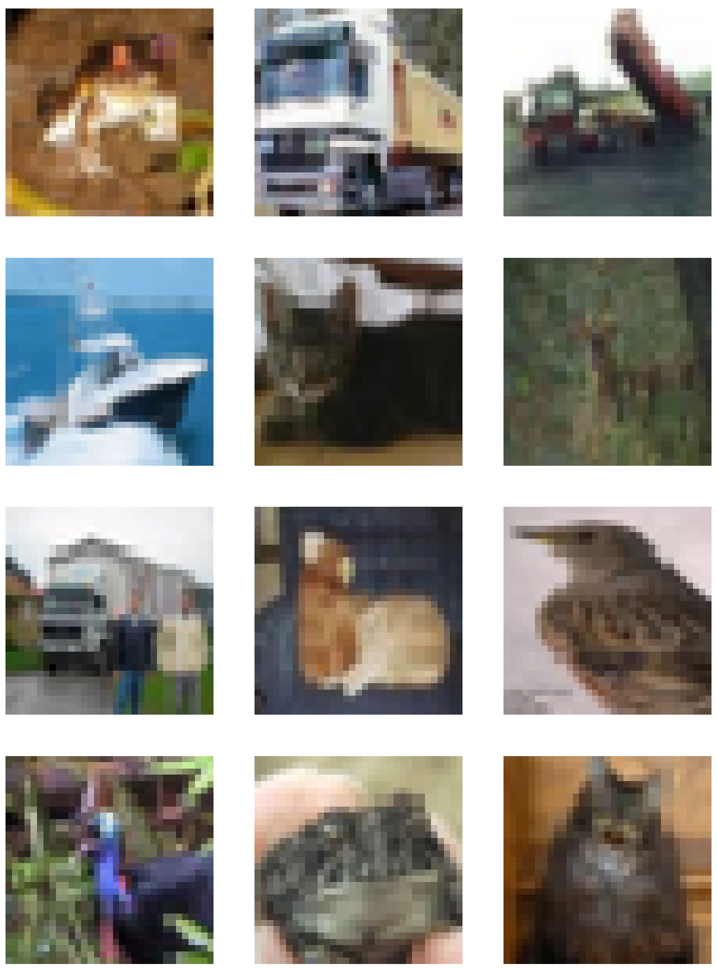


Samples from
Generative Adverserial
[Goodfellow *et al*, 2014]

Diffusion Probabilistic Model Applied to CIFAR-10



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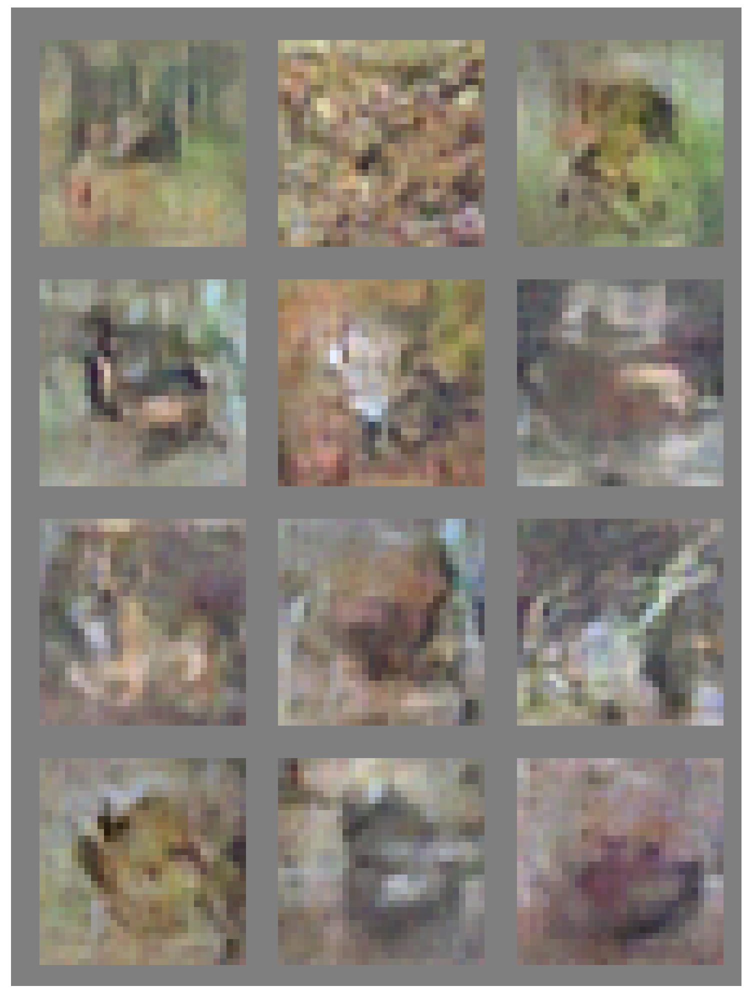

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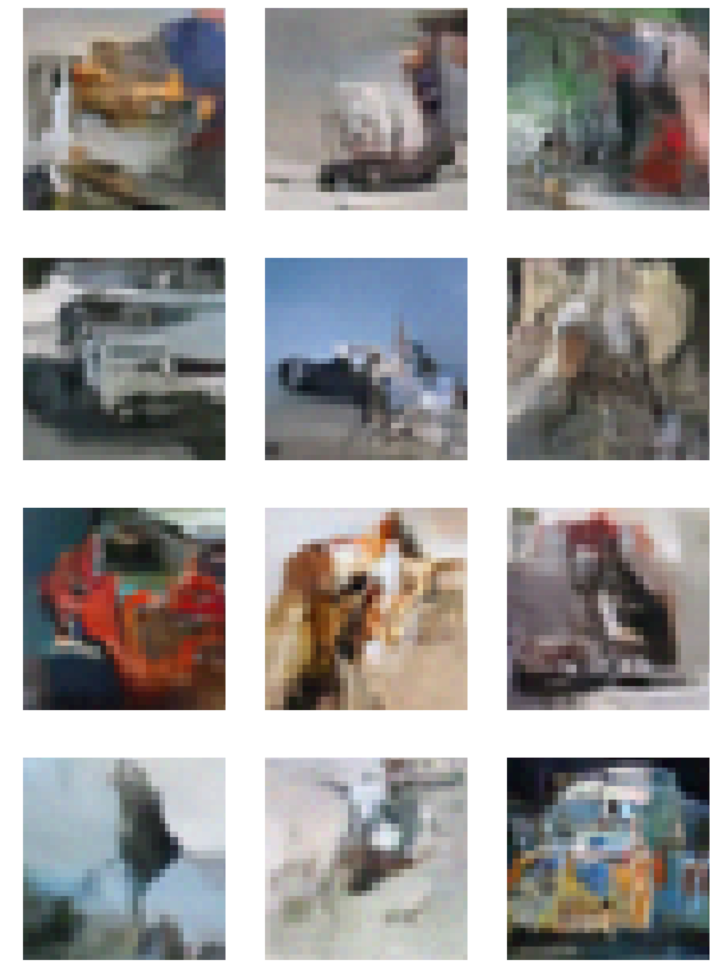
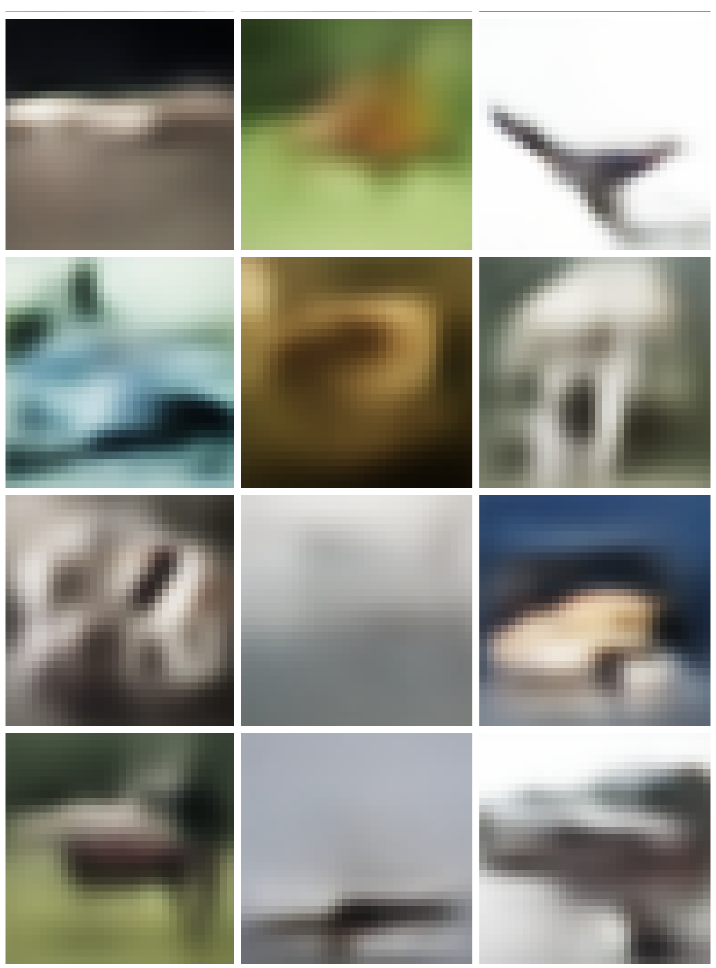
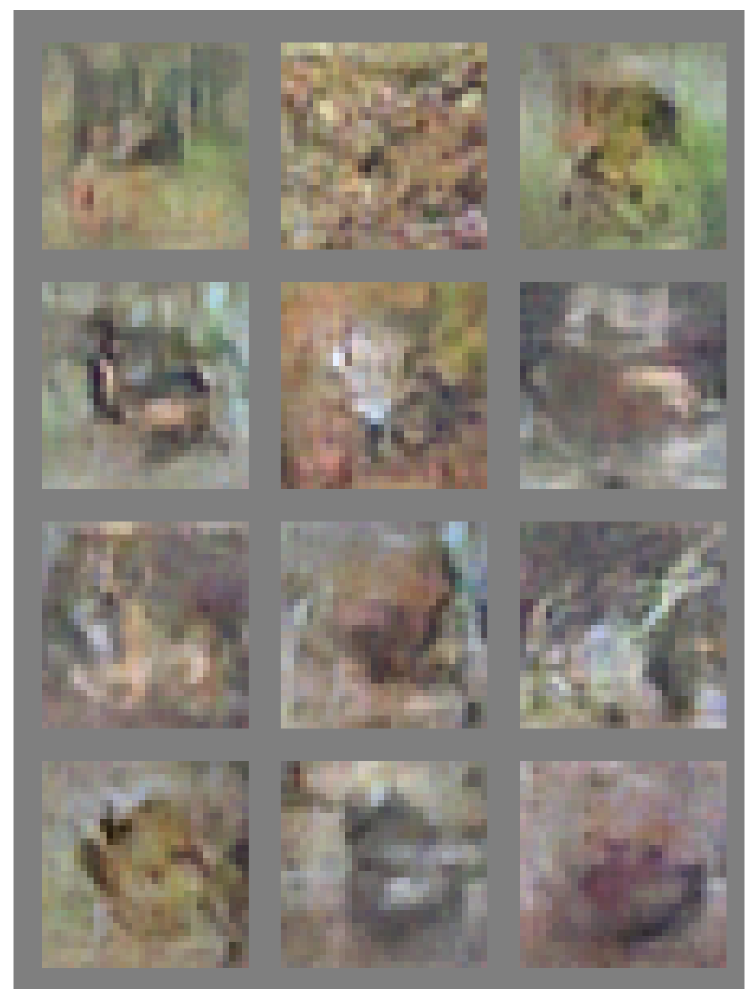


Samples from
diffusion model

Diffusion Probabilistic Model Applied to CIFAR-10



Samples from
DRAW
[Gregor *et al*, 2015]



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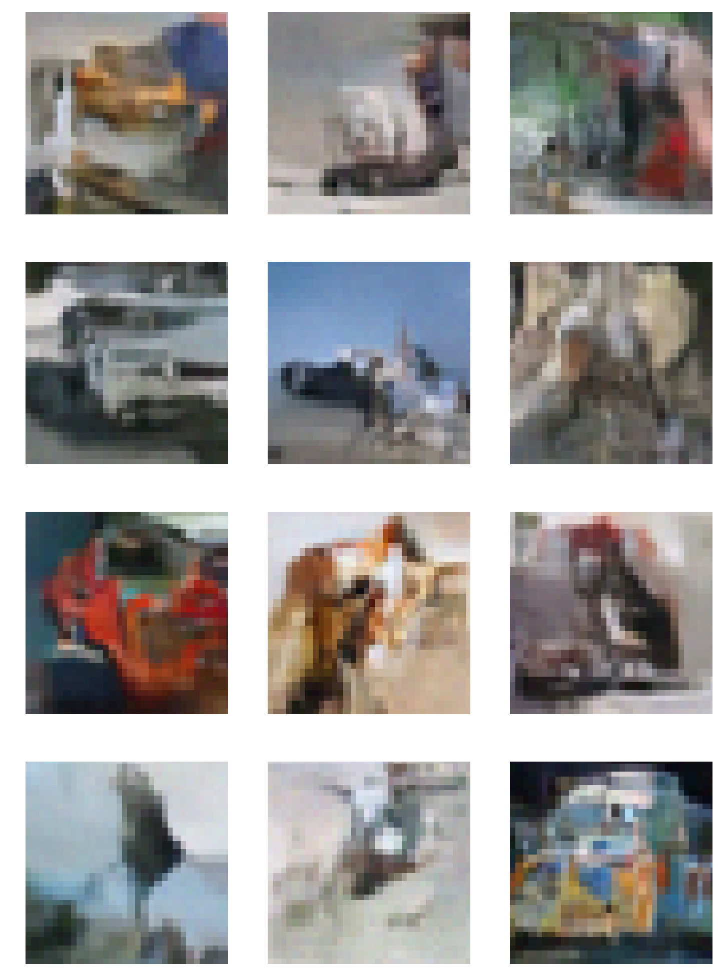

Samples from
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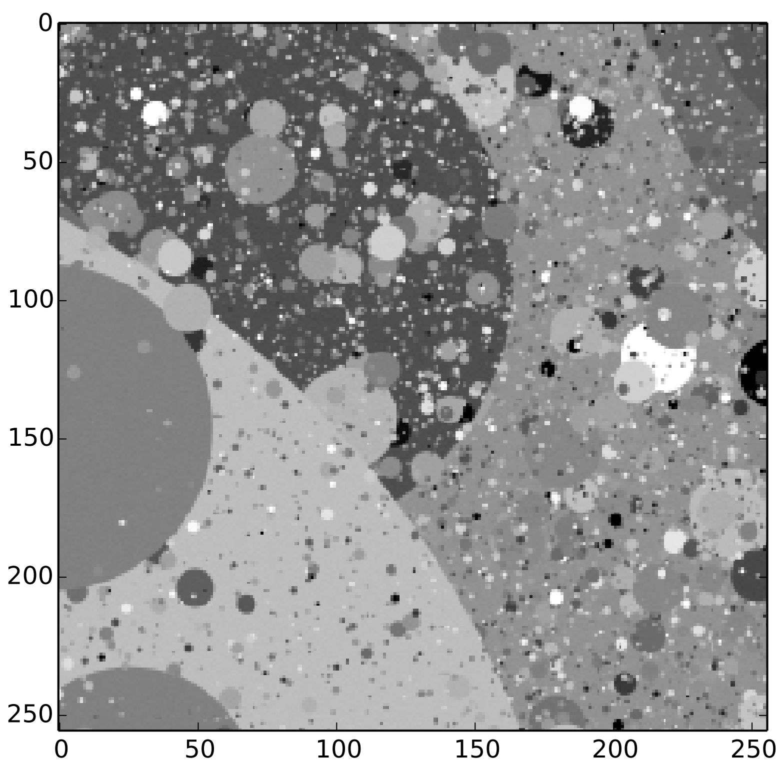
Diffusion Probabilistic Model Applied to Dead Leaves



Training Data

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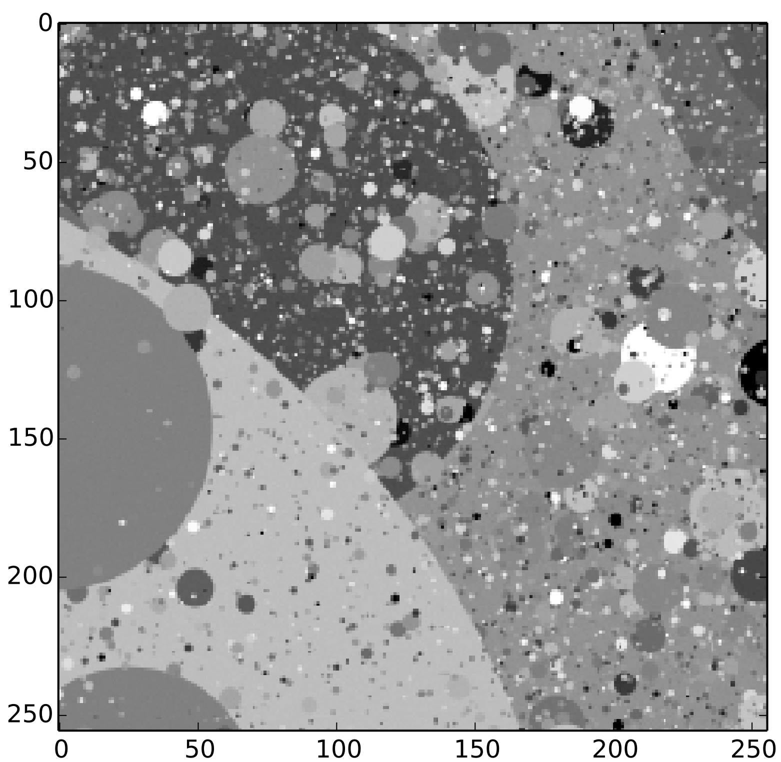
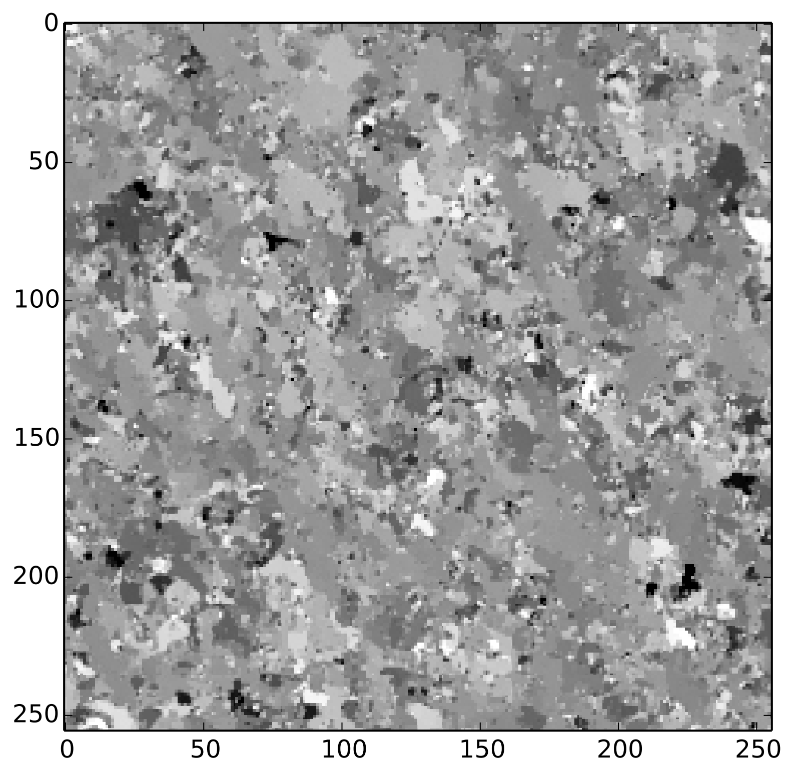
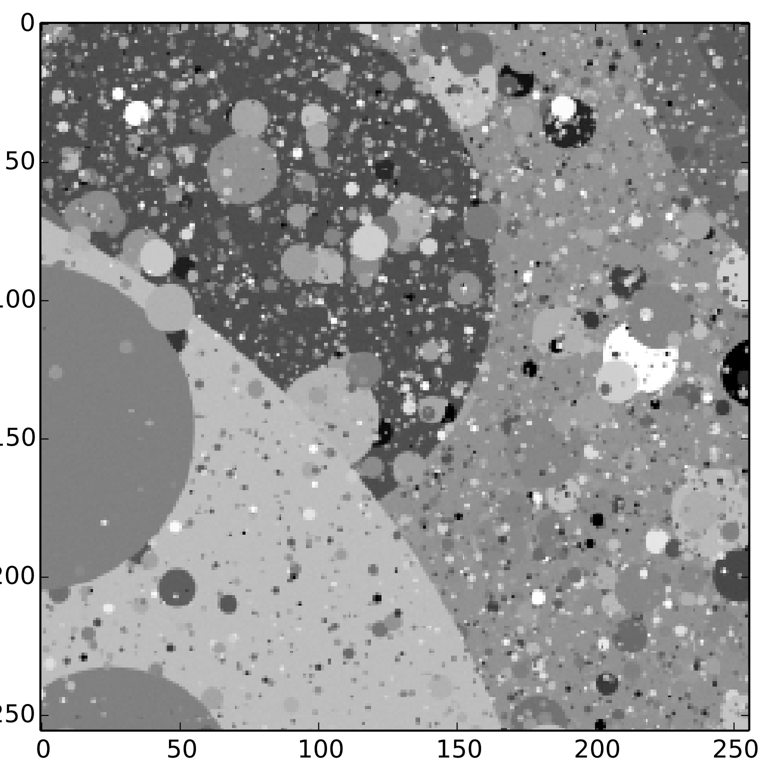


Training Data

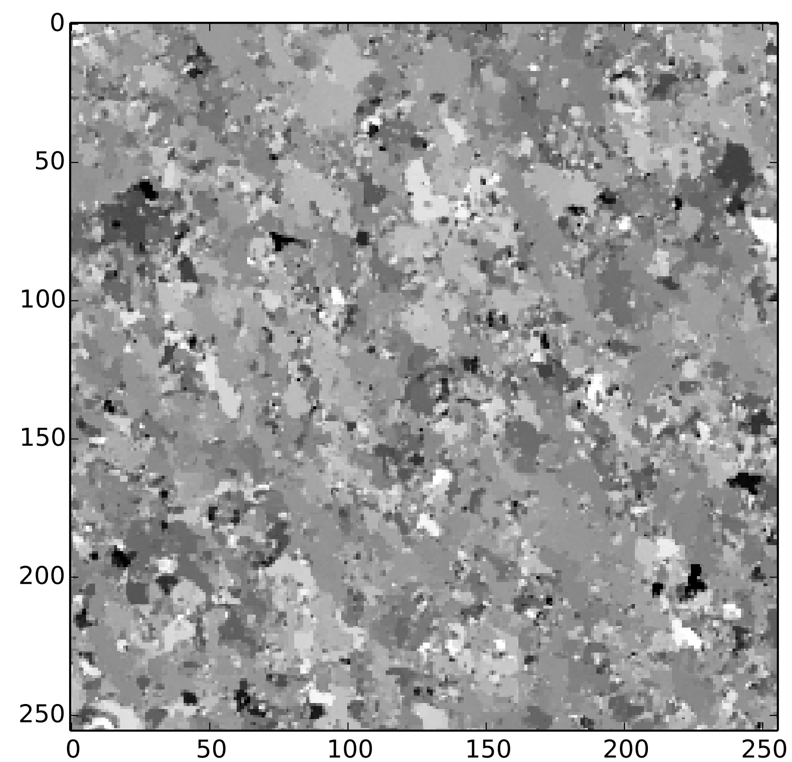


Sample from
[Theis *et al*, 2012]

Diffusion Probabilistic Model Applied to Dead Leaves



Training Data



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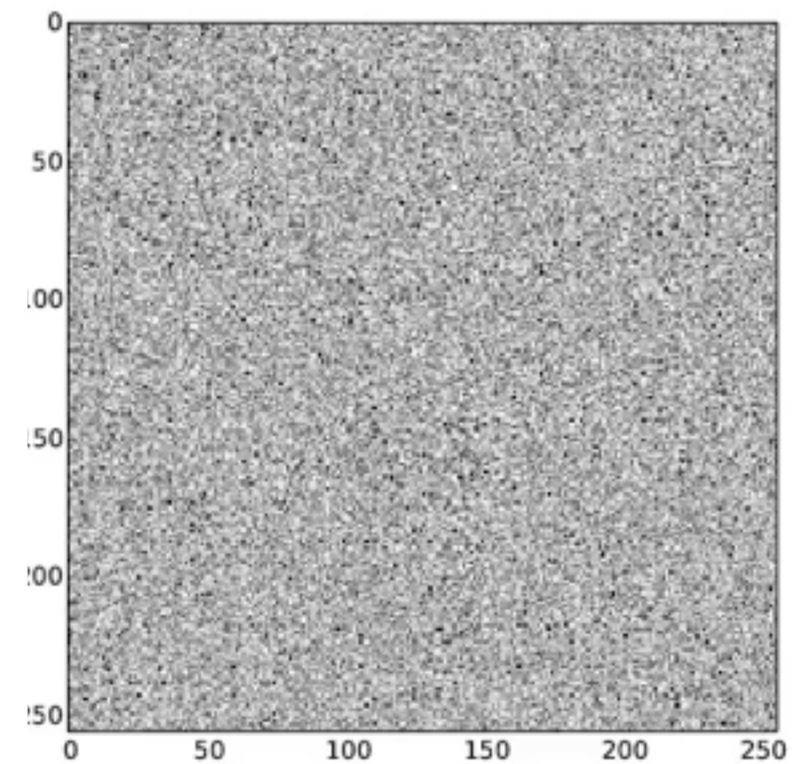

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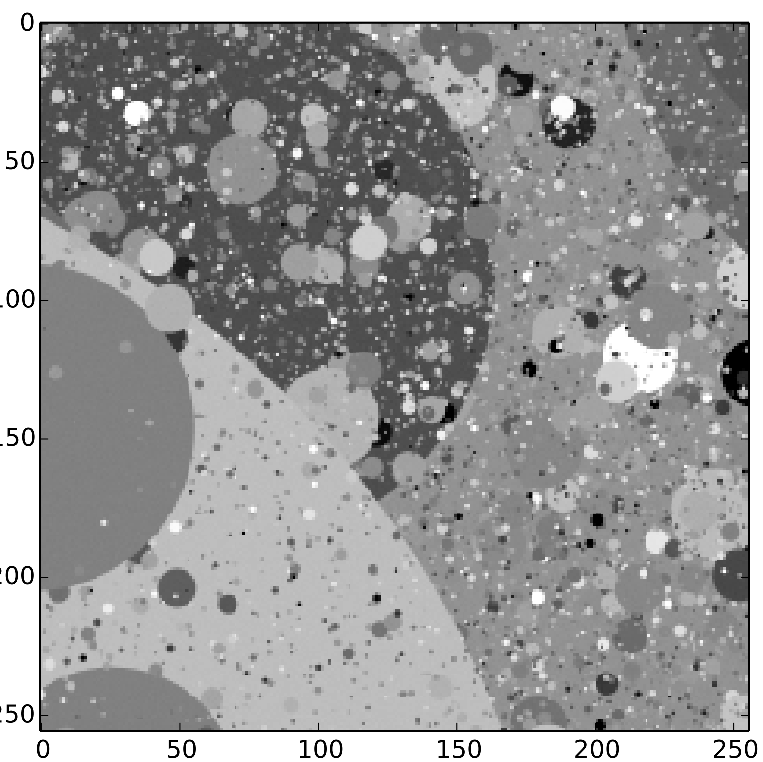

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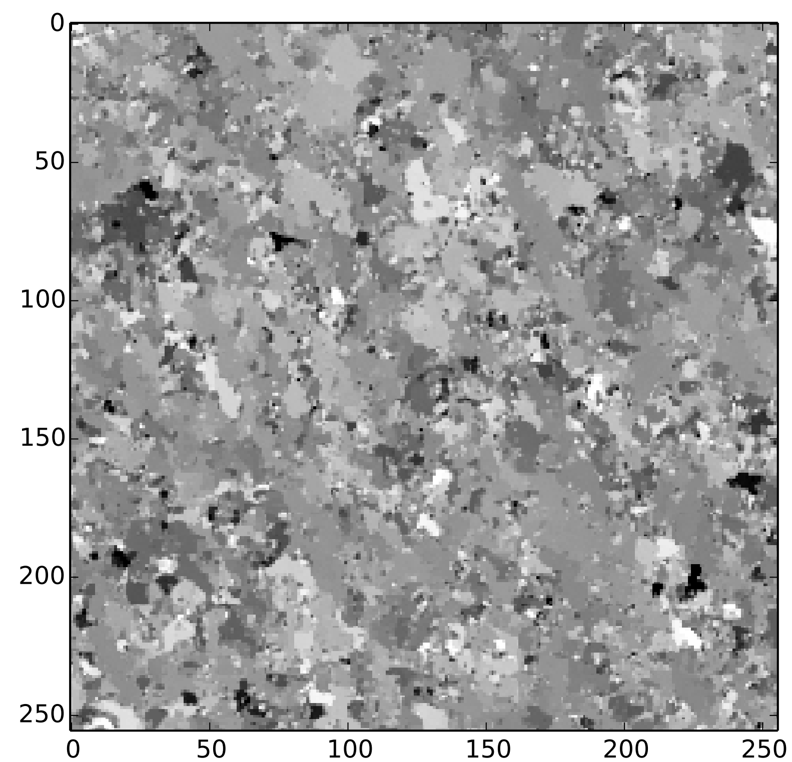

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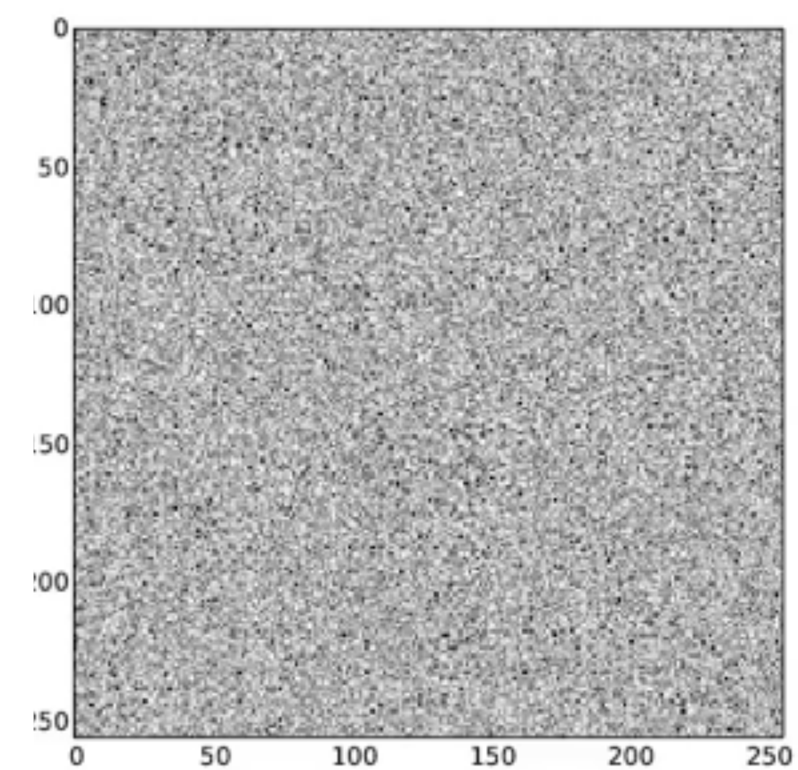

Sample from
diffusion model

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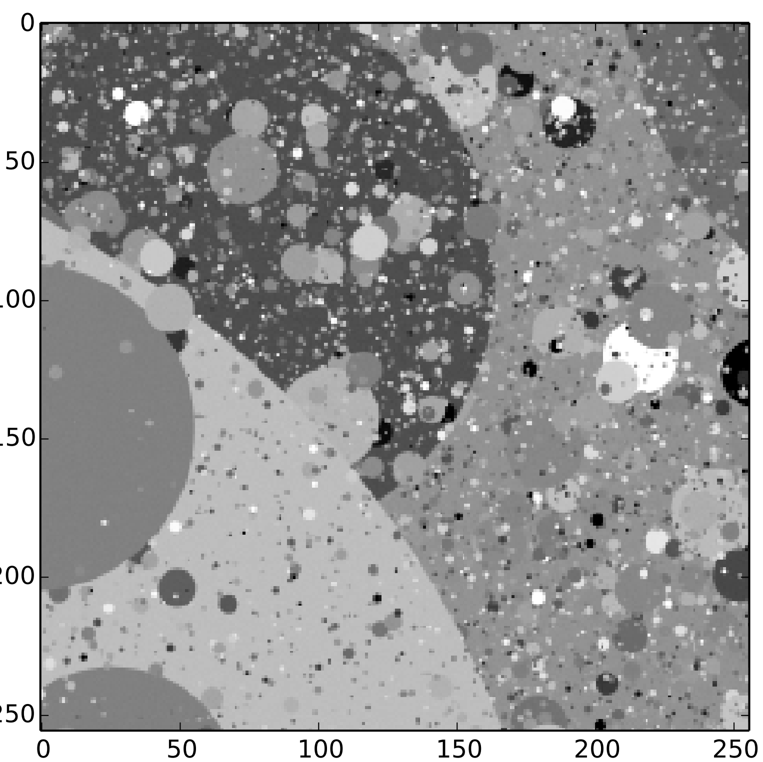
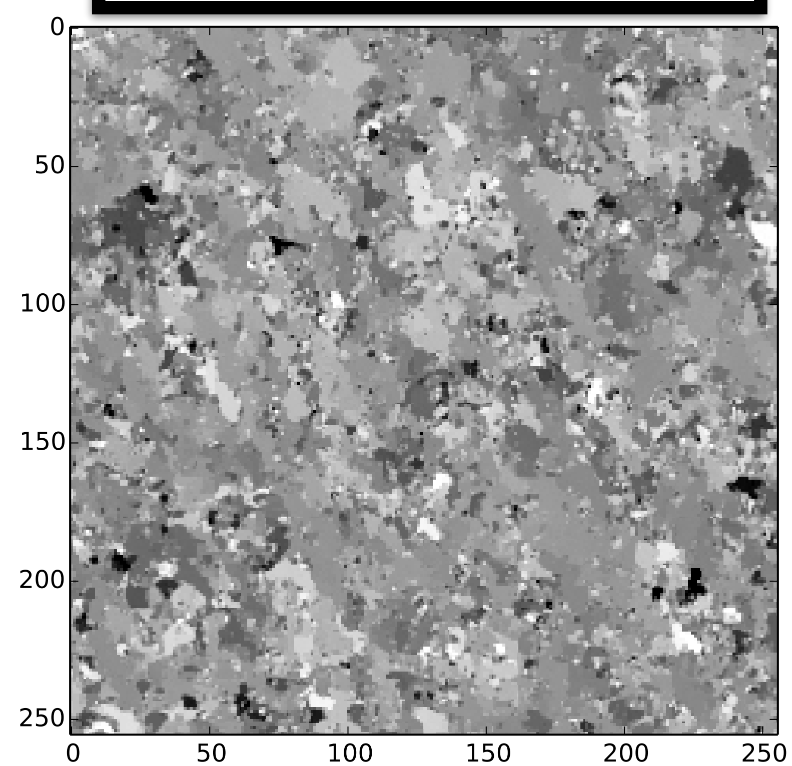


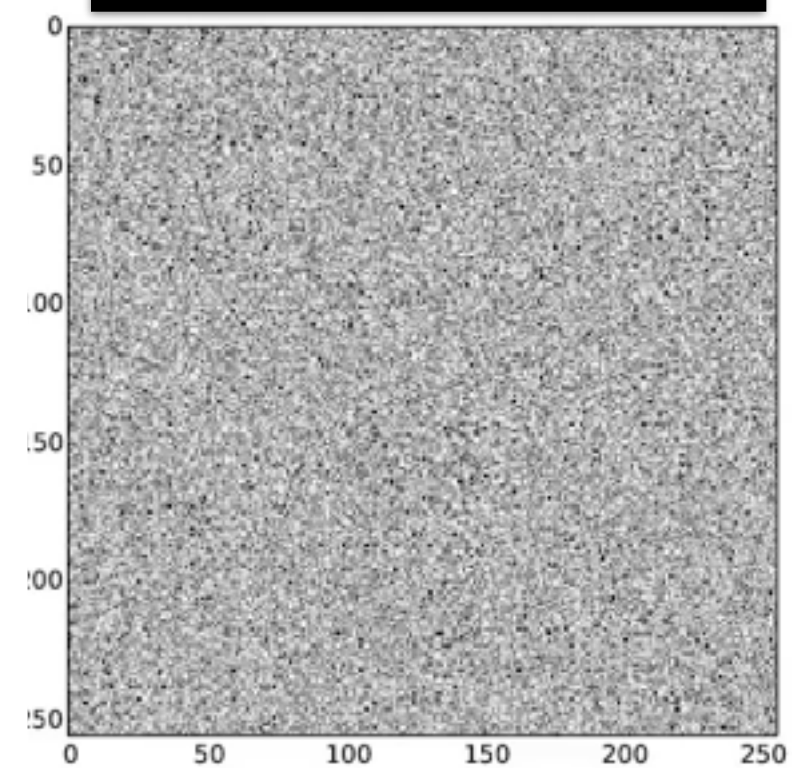
Training Data

Log likelihood
1.24 bits/pixel



Sample from
[Theis *et al*, 2012]

Log likelihood
1.49 bits/pixel



Sample from
diffusion model

Outline

- Motivation: The promise of deep unsupervised learning
- Physical intuition: Diffusion processes and time reversal
- Diffusion probabilistic model: Derivation and experimental results
    - Algorithm
    - Deep convolutional network: Universal function approximator
    - **Multiplying distributions: Inputation, denoising, computing posteriors**
- Other projects: Training energy based models, Monte Carlo, deep learning theory

Multiplying Distributions is Straightforward

Interested in $\tilde{p}\left(\mathbf{x}^{(0)}\right) \propto p\left(\mathbf{x}^{(0)}\right) r\left(\mathbf{x}^{(0)}\right)$

- Required to compute posterior distributions
  - Missing data (inpainting)
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- Required to compute posterior distributions
  - Missing data (inpainting)
  - Corrupted data (denoising)
- Difficult and expensive using competing techniques
  - e.g. VAEs, GSNs, NADEs, GANs, RNVP, most graphical models

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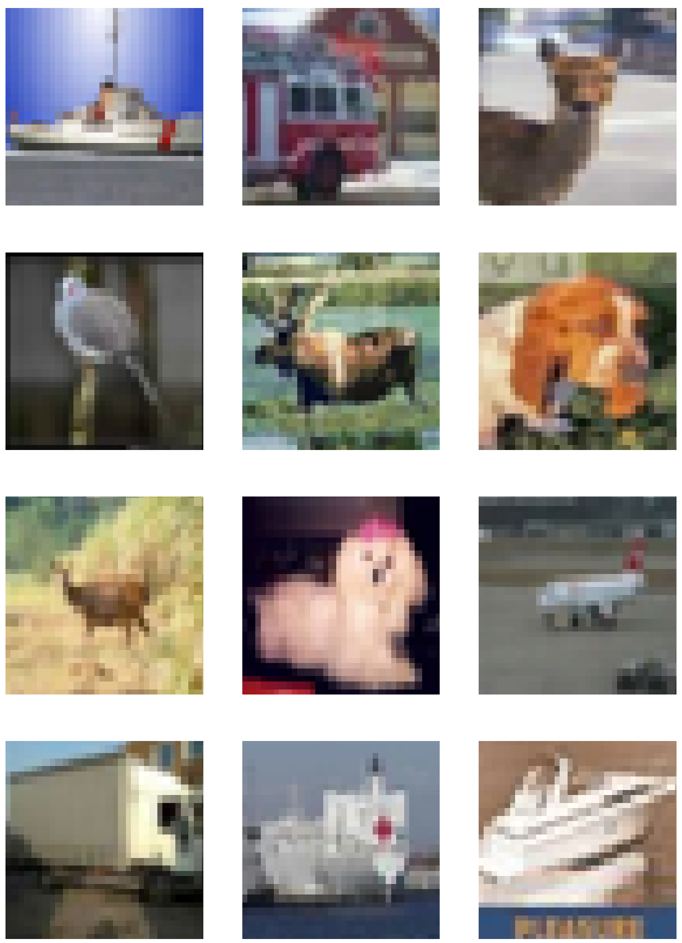
Acts as small perturbation to diffusion process

$$p\left(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}\right) = \mathcal{N}\left(\mathbf{x}^{(t-1)}; f_{\mu}\left(\mathbf{x}^{(t)}, t\right), f_{\Sigma}\left(\mathbf{x}^{(t)}, t\right)\right)$$

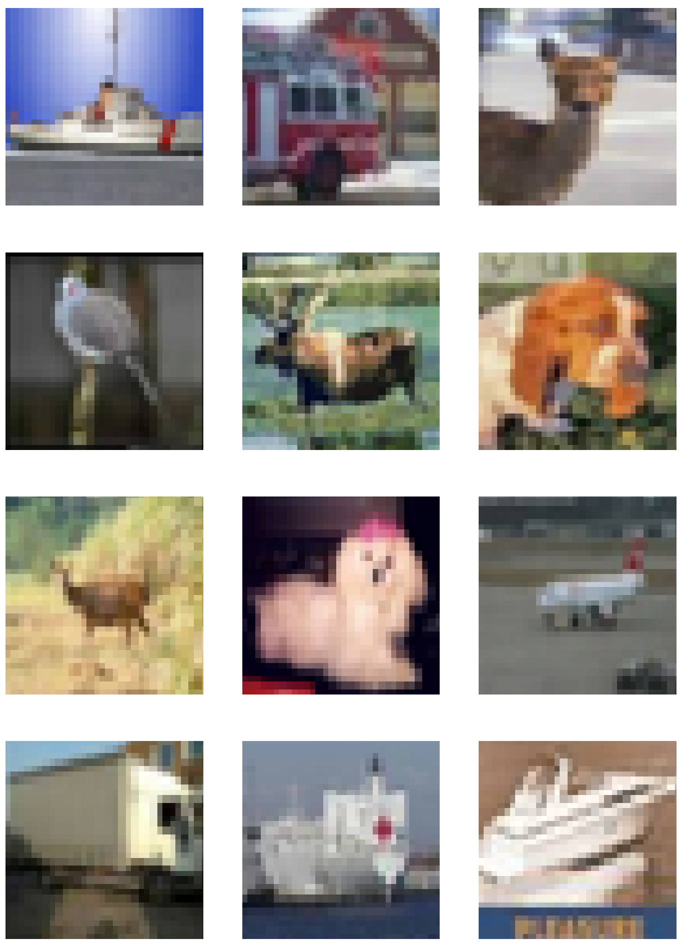
$$\tilde{p}\left(\mathbf{x}^{(t-1)} \mid \mathbf{x}^{(t)}\right) \approx \mathcal{N}\left(x^{(t-1)}; \mathbf{f}_{\mu}\left(\mathbf{x}^{(t)}, t\right) + \mathbf{f}_{\Sigma}\left(\mathbf{x}^{(t)}, t\right) \left.\frac{\partial \log r\left(\mathbf{x}^{(t-1)'}\right)}{\partial \mathbf{x}^{(t-1)'}}\right|_{\mathbf{x}^{(t-1)'}=f_{\mu}\left(\mathbf{x}^{(t)}, t\right)}, \mathbf{f}_{\Sigma}\left(\mathbf{x}^{(t)}, t\right)\right)$$

Image Denoising by Sampling from Posterior



Holdout Data

Image Denoising by Sampling from Posterior



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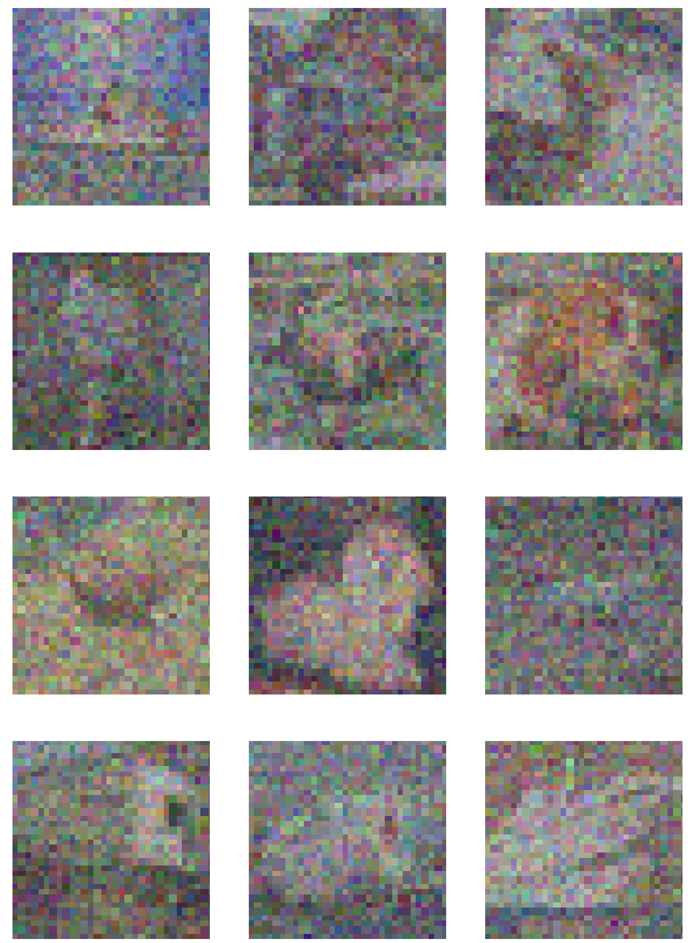
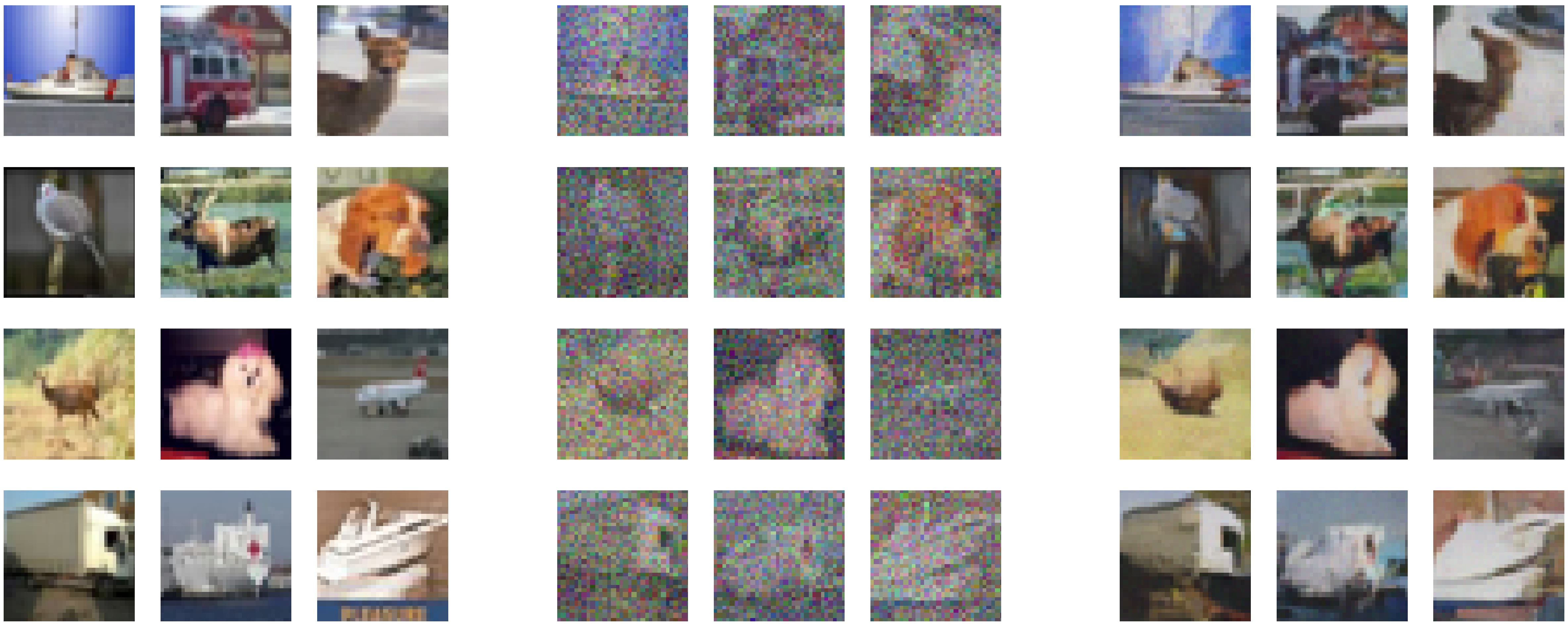


Corrupted
(SNR = 1)

Image Denoising by Sampling from Posterior



Holdout Data | Corrupted (SNR = 1) | Denoised

Image Inpainting by Sampling from Posterior

- Training data [Lazebnik *et al*, 2005]

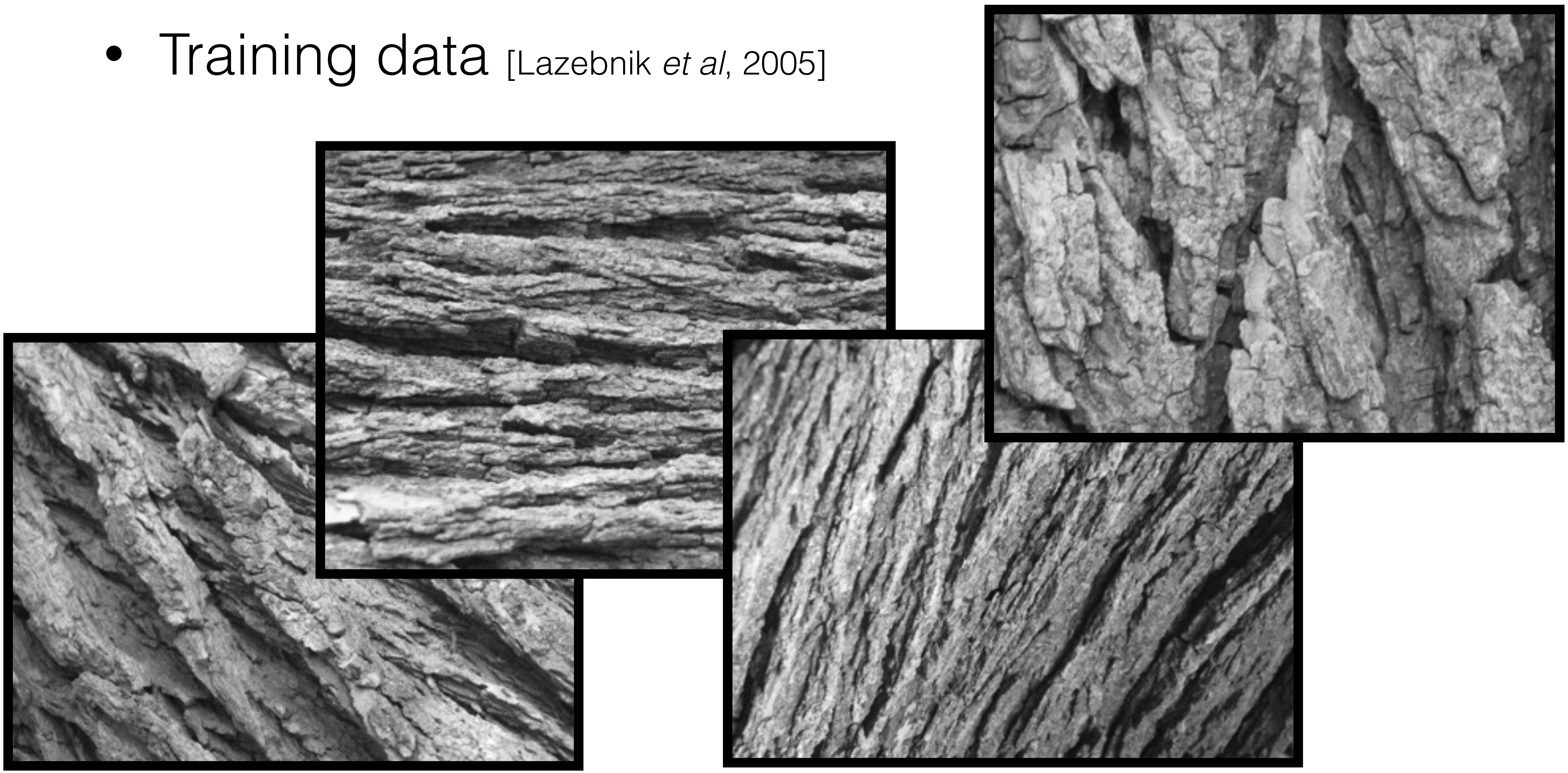
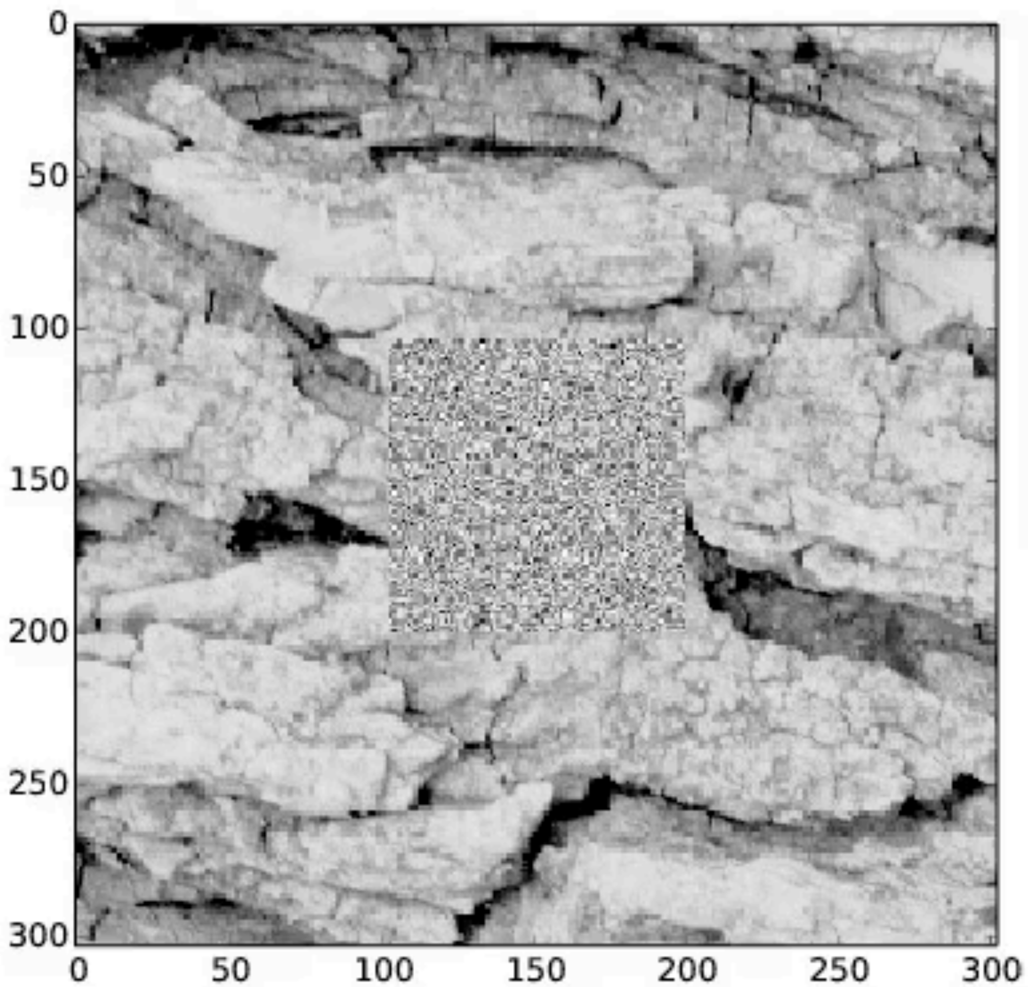
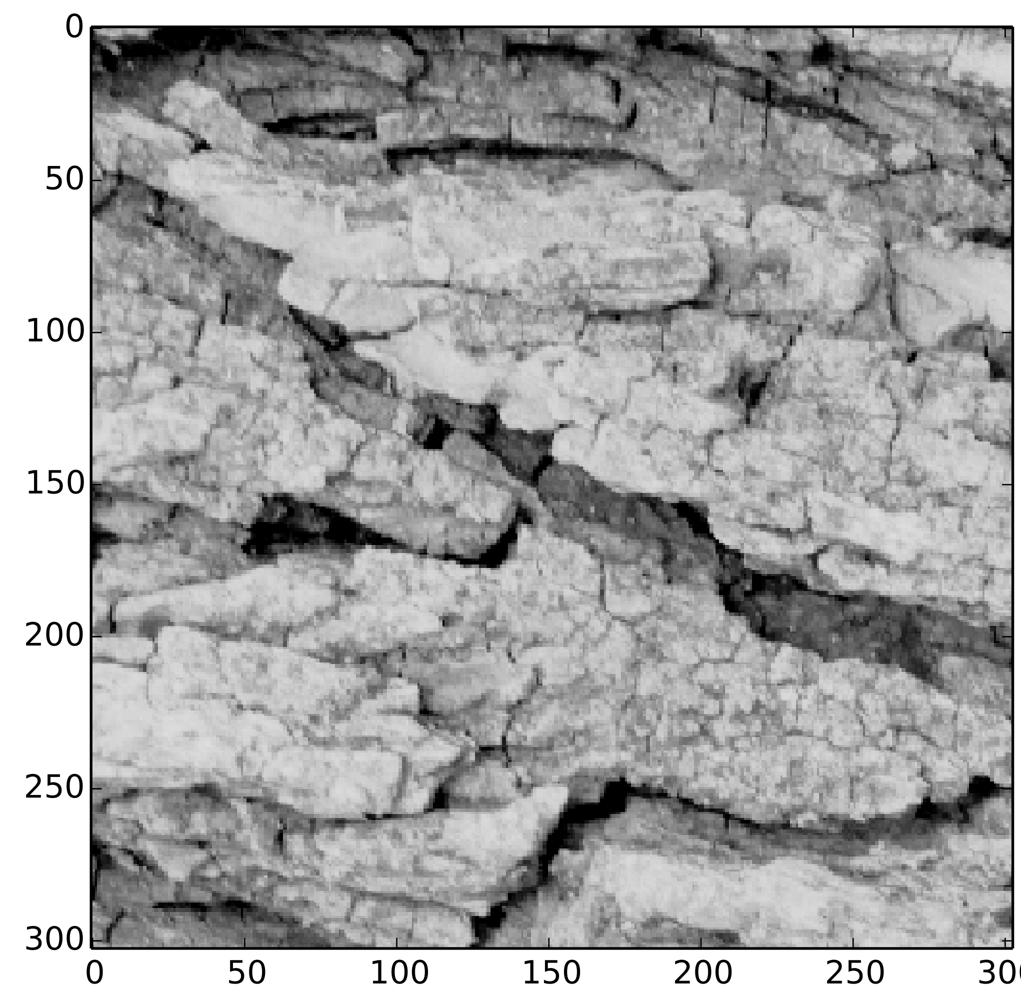


Image Inpainting by Sampling from Posterior

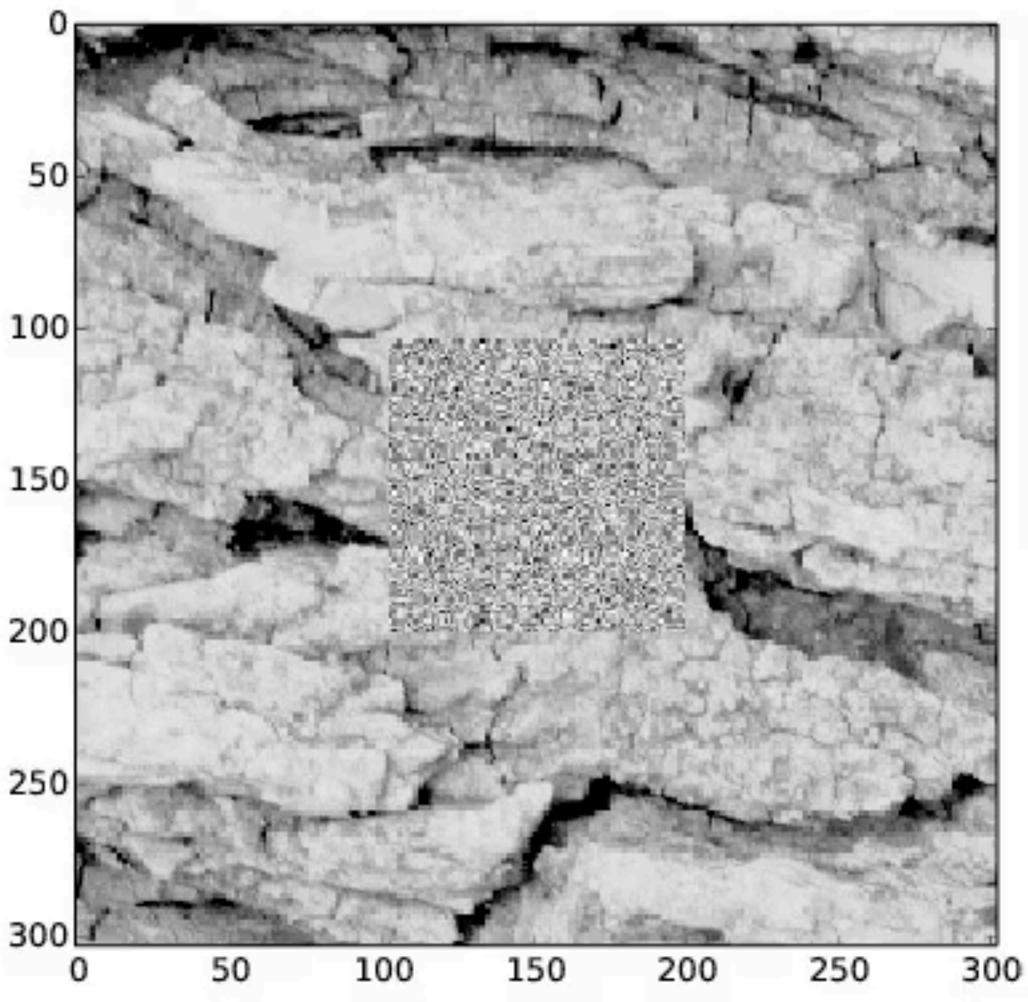


Inpainted image

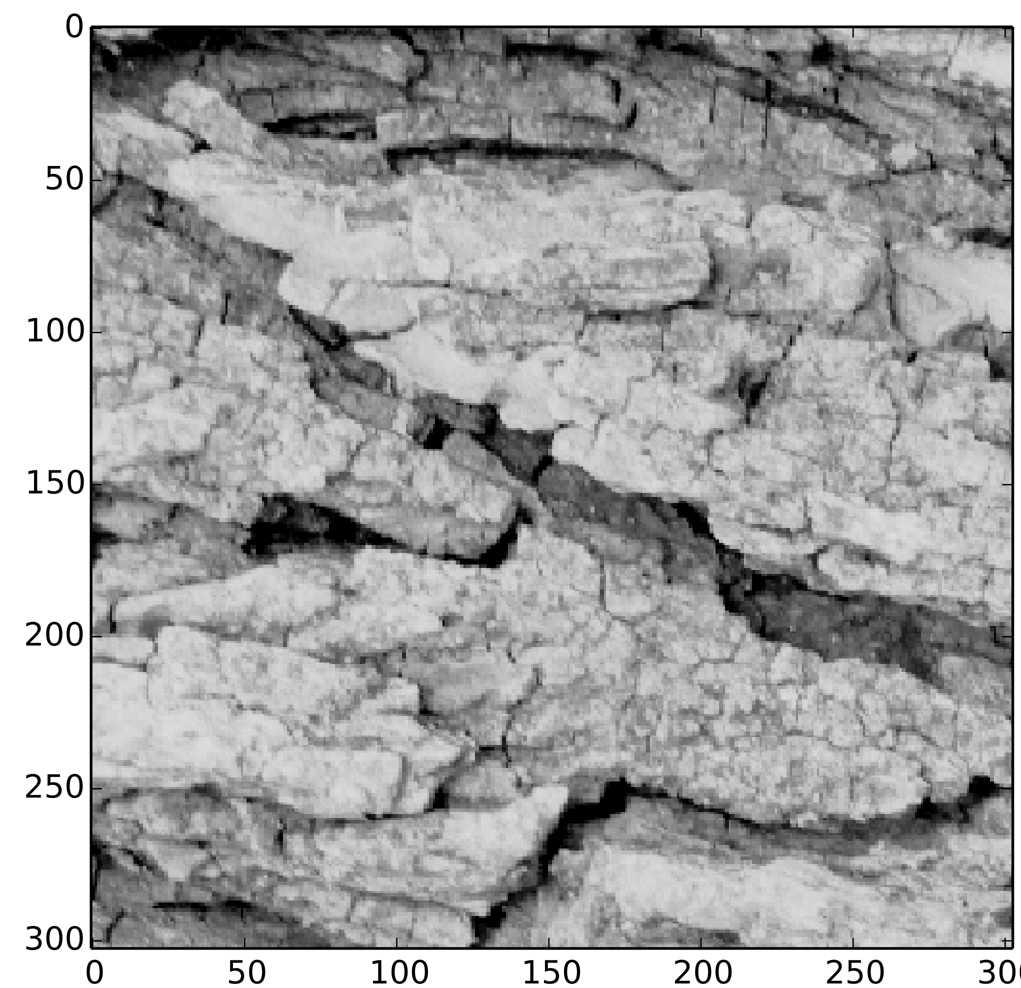


True image

Image Inpainting by Sampling from Posterior



Inpainted image



True image

Flexible and tractable method for deep unsupervised learning

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- Easy to multiply distributions (e.g. for posterior)
- Bounds on entropy production

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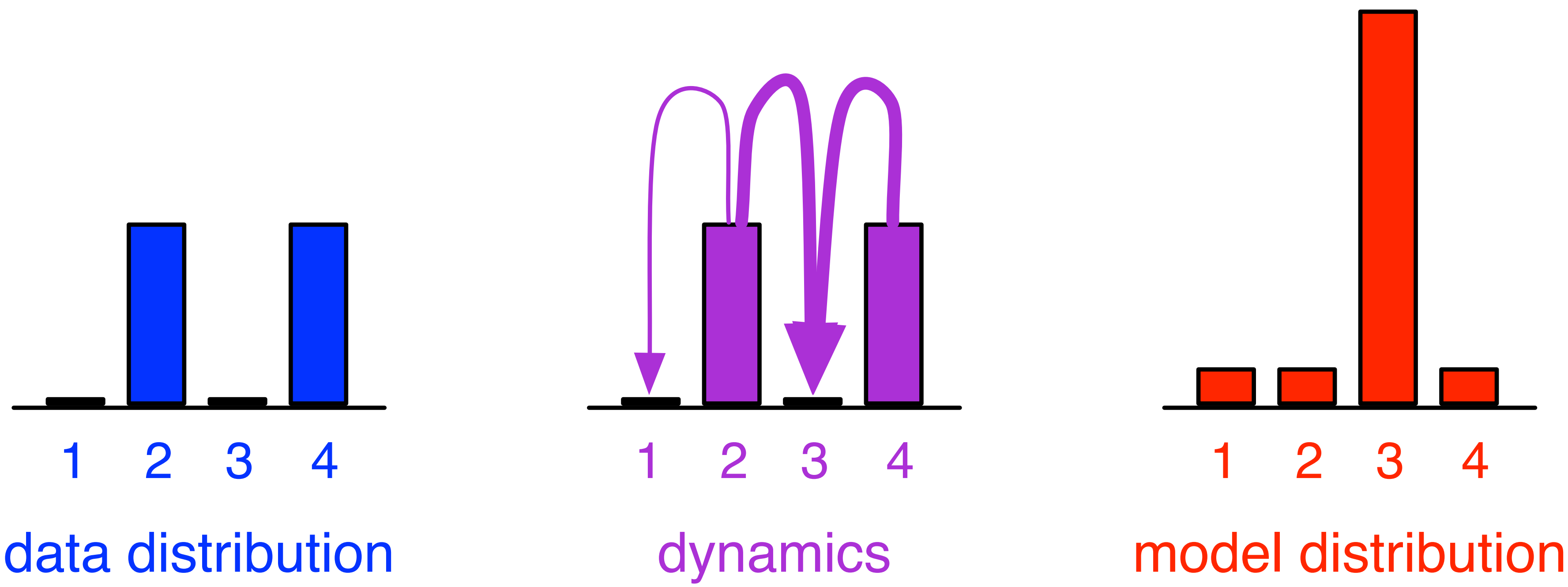
Minimum Probability Flow Learning

- Estimate parameters in energy based models, by minimizing probability flow under master equation from stat. mech.



$$p_i^{(0)} = \text{fraction data in state } i$$

$$p_i^{(\infty)}(\theta) = \frac{e^{-E_i(\theta)}}{Z(\theta)}$$

$$\dot{p}_i^{(t)} = \sum_{j \neq i} \Gamma_{ij}(\theta)\, p_j^{(0)} - \sum_{j \neq i} \Gamma_{ji}(\theta)\, p_i^{(0)}$$

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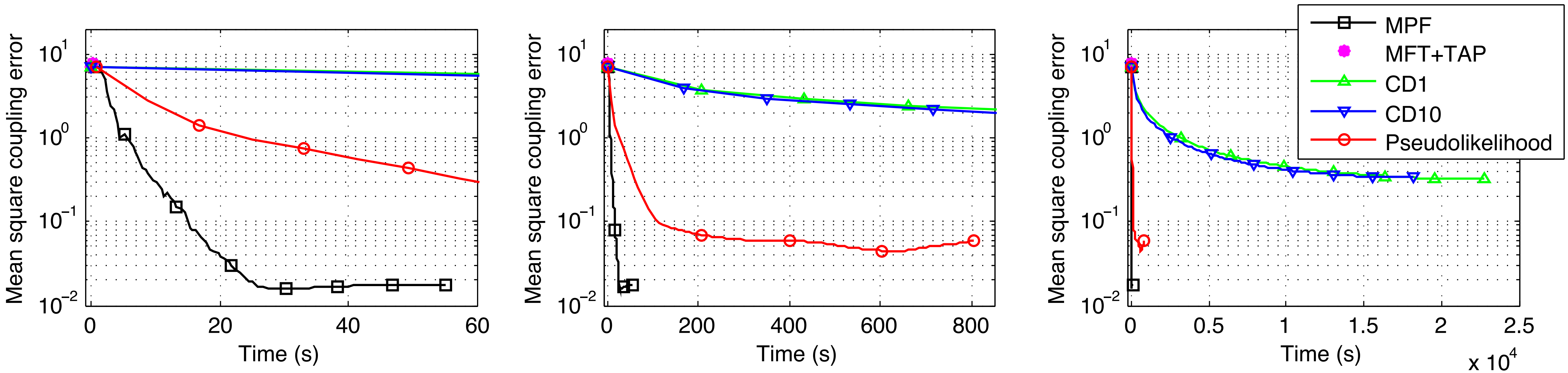
$$\dot{p}_i^{(\infty)} = 0$$

[PRL, 2011]
[ICML, 2011]

Minimum Probability Flow Learning

- More rapidly solves inverse Ising problem

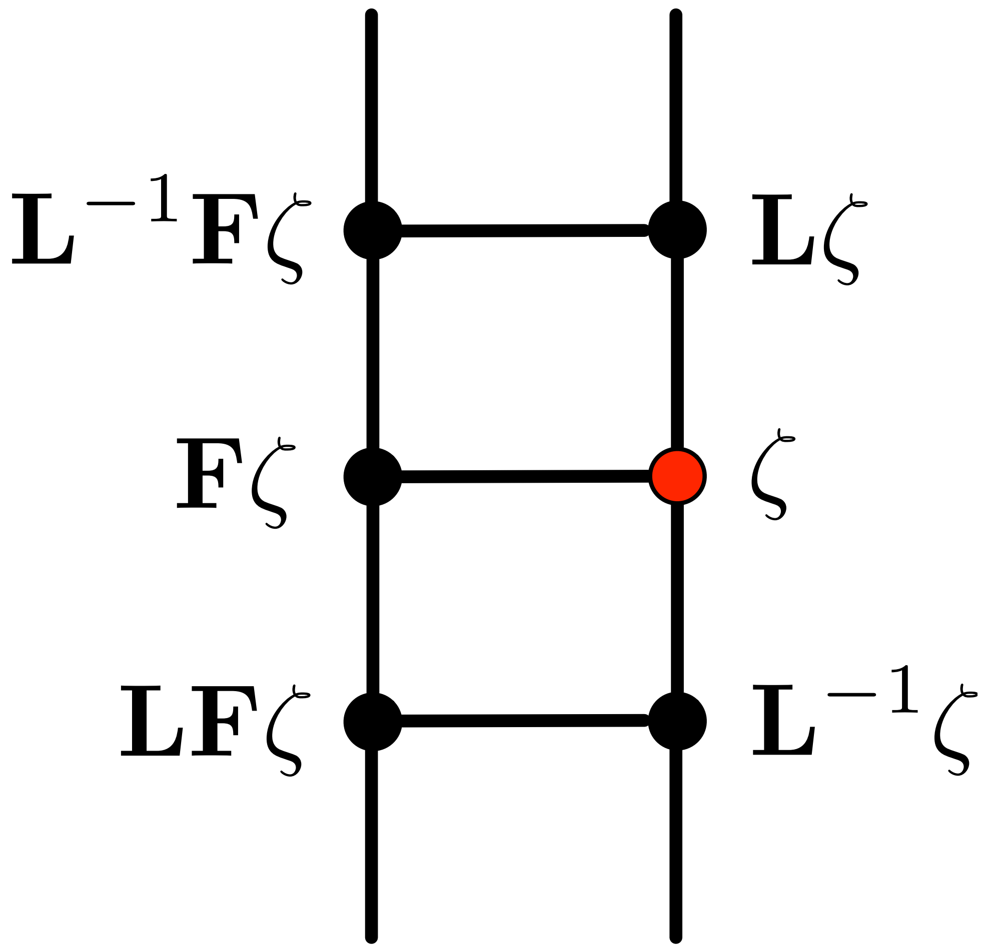


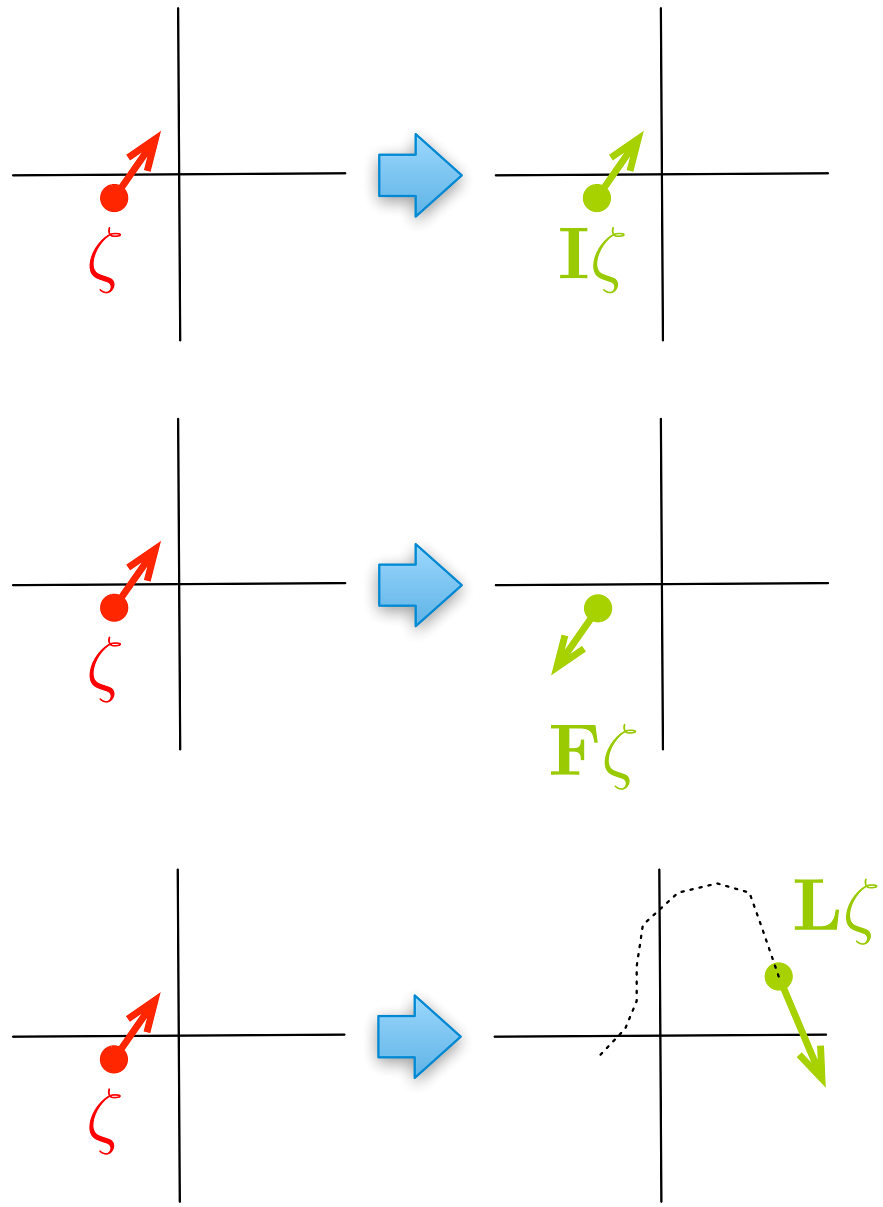
First 60 seconds | First 800 seconds | First 25,000 seconds

[PRL, 2011]
[ICML, 2011]

Hamilton Monte Carlo Without Detailed Balance

- Describe HMC using operators on discrete state space

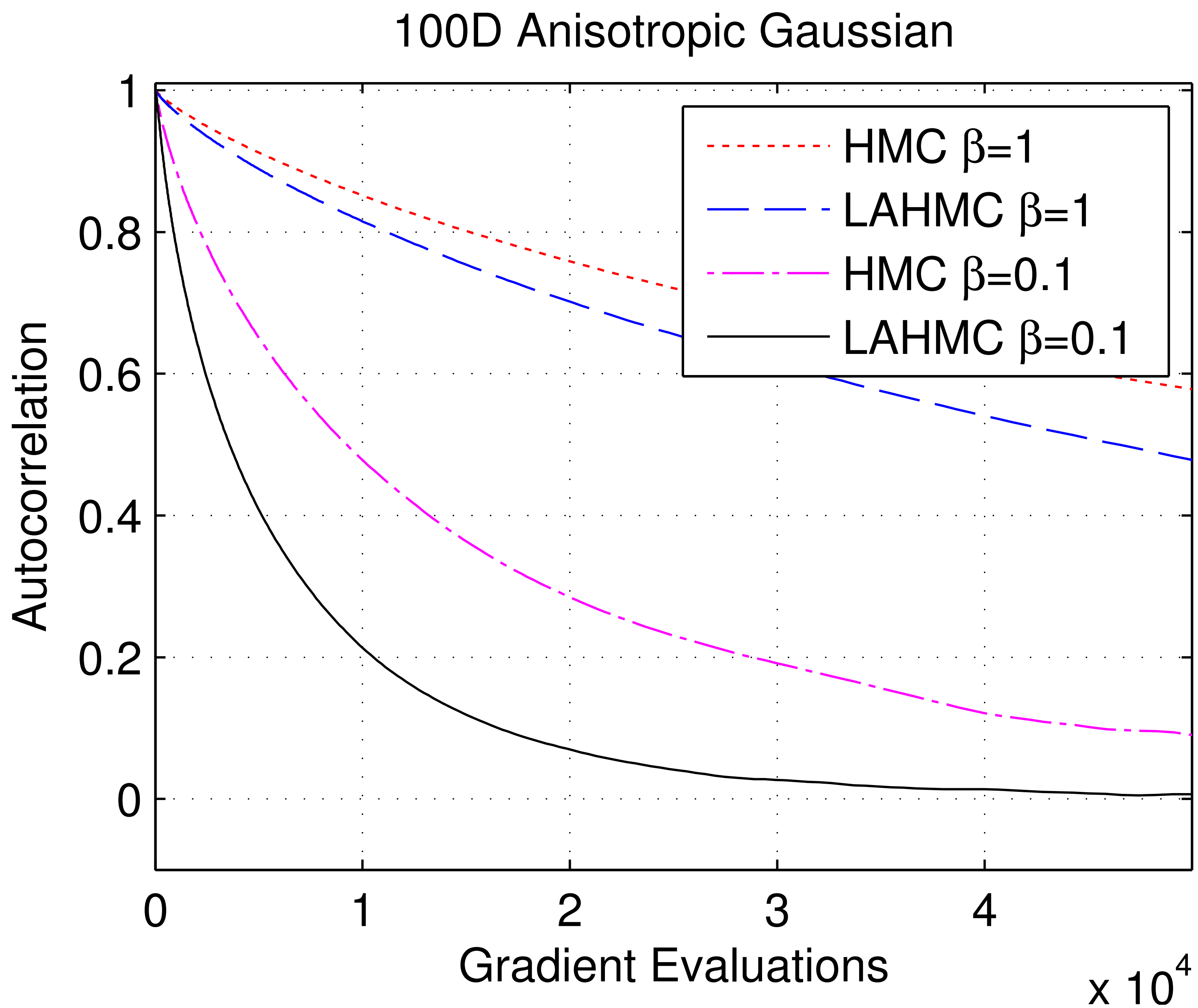




[ICML, 2014]

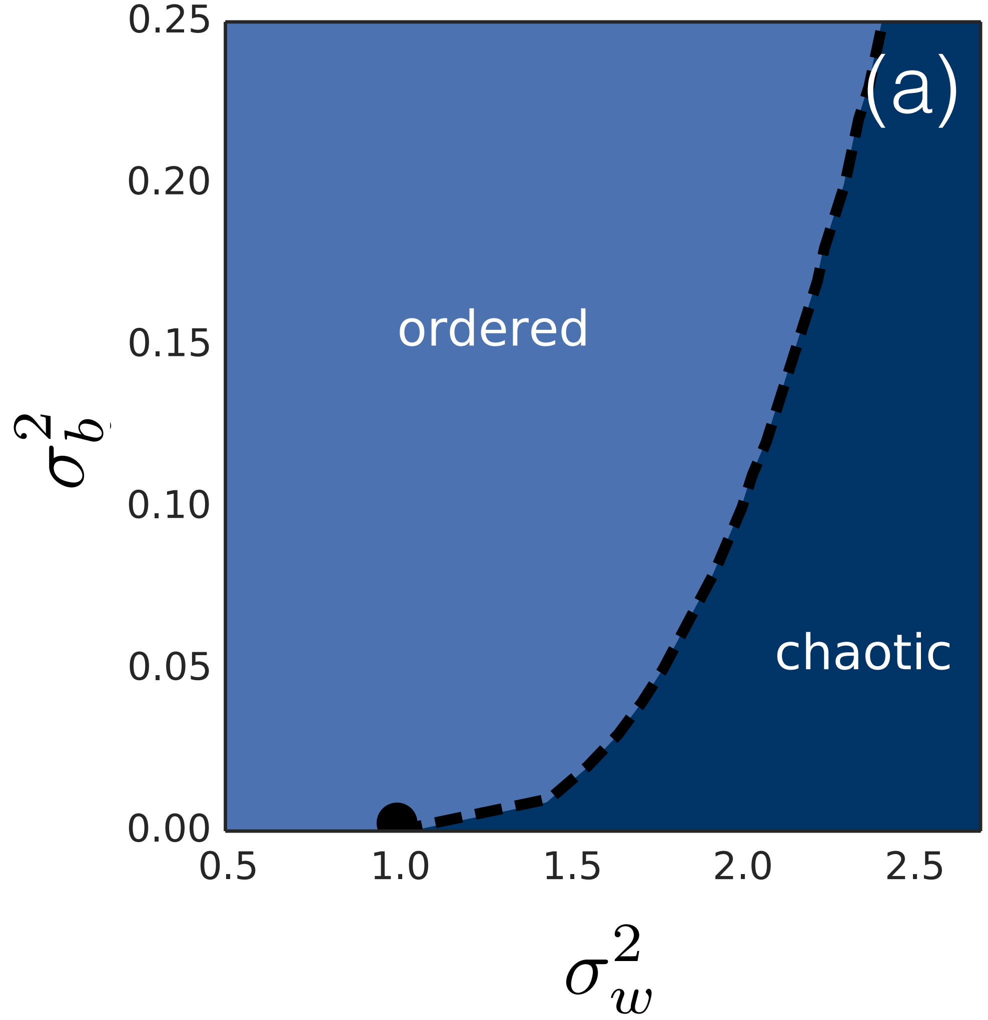
Hamiltonian Monte Carlo Without Detailed Balance

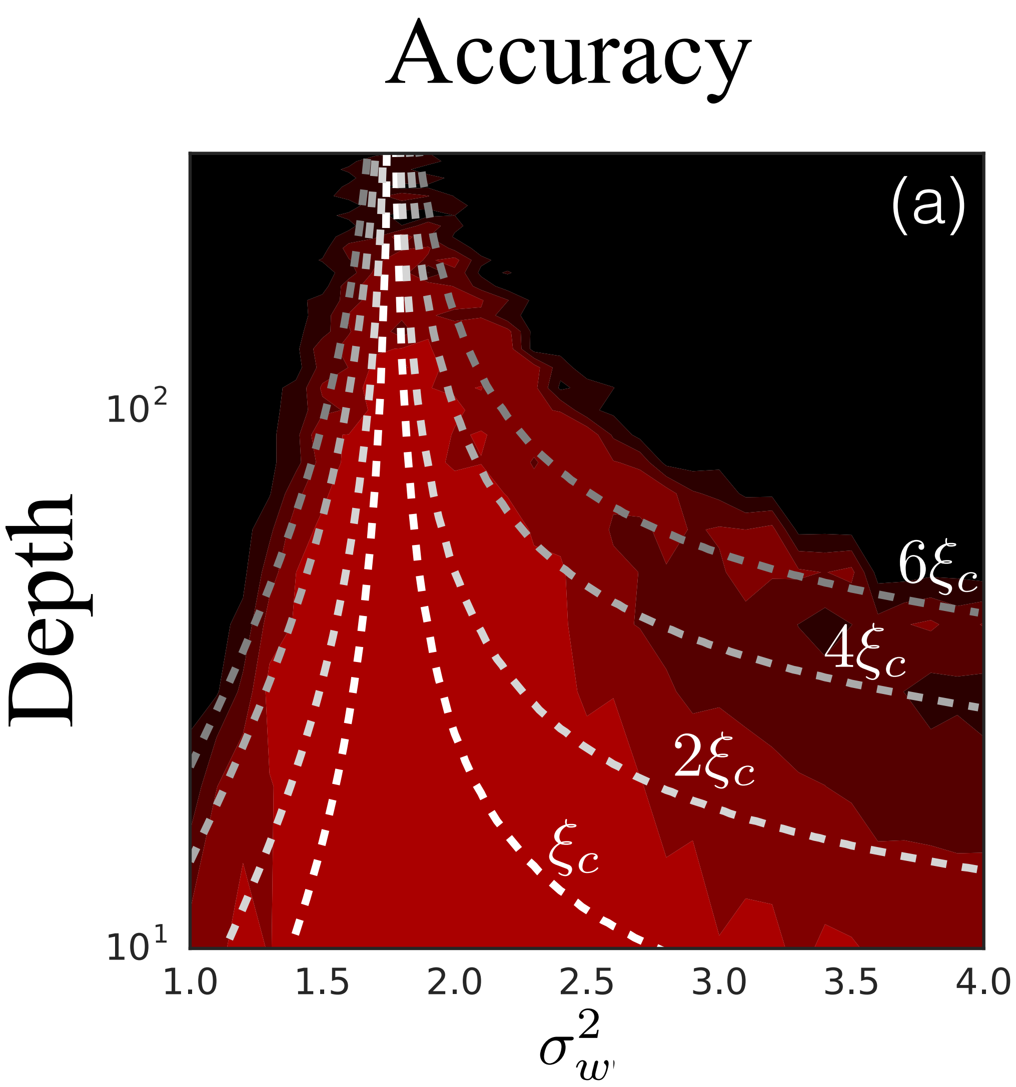
- Improved mixing by violating detailed balance



[ICML, 2014]

Predict properties of deep networks using mean field theory





[NIPS, 2016]
[ICLR, 2017 (under review)]

Thanks!

Collaborators

Eric
Weiss

Niru
Maheswaranathan

Surya
Ganguli

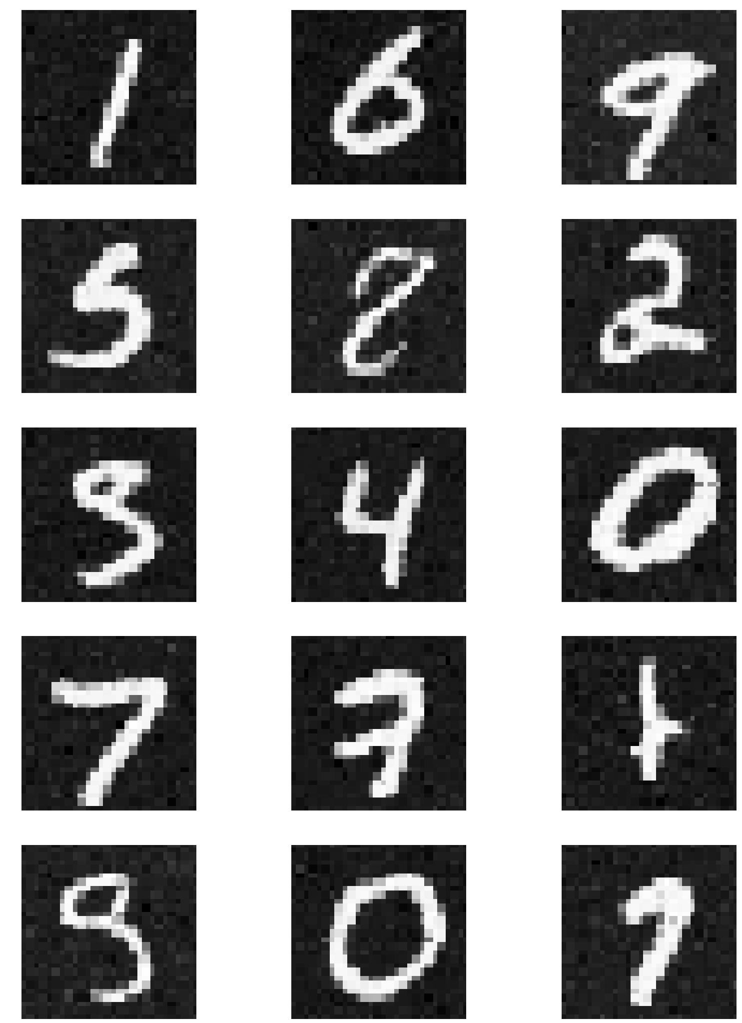
Endless discussion

- The Ganguli Gang
- The Redwood Center for Theoretical Neuroscience
- Google Brain

Diffusion Probabilistic Model Applied to MNIST

Model	**Log likelihood estimate***
Stacked CAE	121 ± 1.6 bits
DBN	138 ± 2 bits
Deep GSN	214 ± 1.1 bits
Diffusion	**220 ± 1.9 bits**
Adversarial net	225 ± 2 bits

* via Parzen window code from [Goodfellow *et al*, 2014]



Samples from diffusion model

Future Work

Future Work

- Continuous time formulation

Future Work

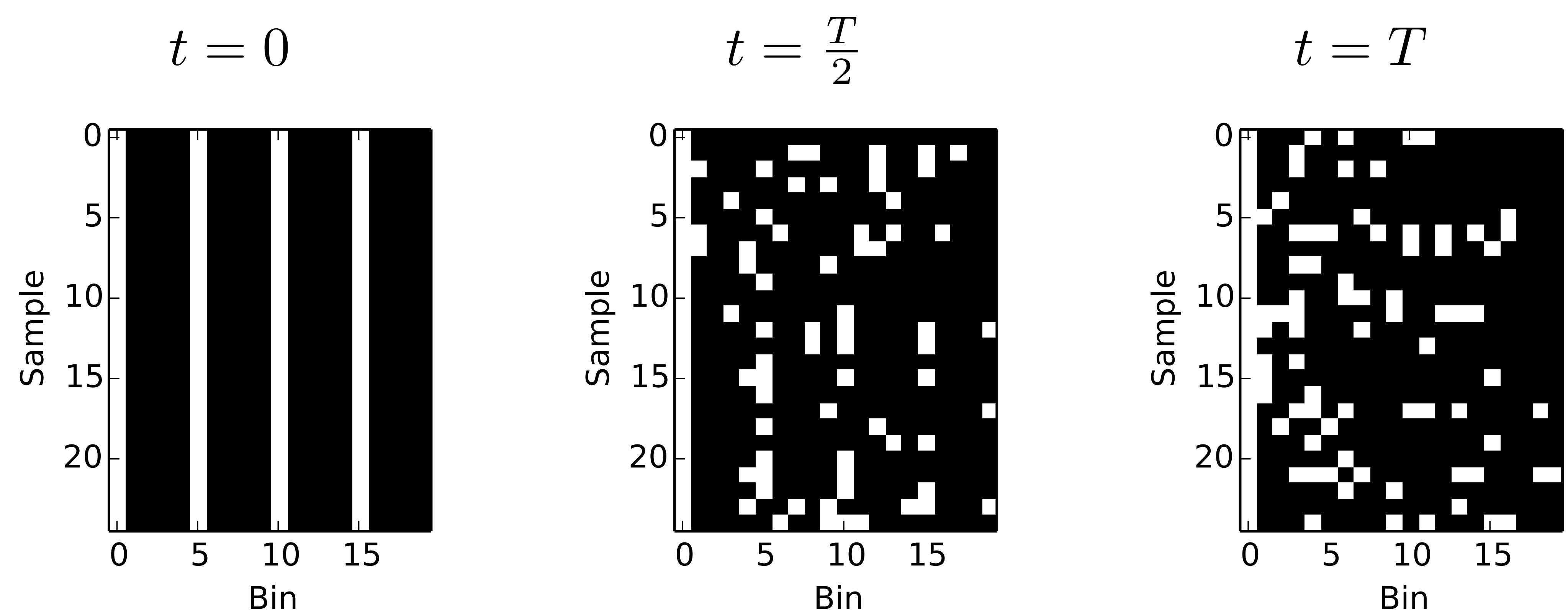
- Continuous time formulation
- Perturbation around energy based model

Future Work

- Continuous time formulation
- Perturbation around energy based model
- Binary data (e.g. spike trains)

Toy Binary Sequence Learning

$$p\left(\mathbf{x}^{(0\cdots T)}\right)$$



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- Extremely flexible, parametric, function approximation

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- **Single layer:** linear transformation, pointwise nonlinearity

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$$\mathbf{y}^l = \sigma\left(\mathbf{W}^l \mathbf{y}^{l-1}\right)$$

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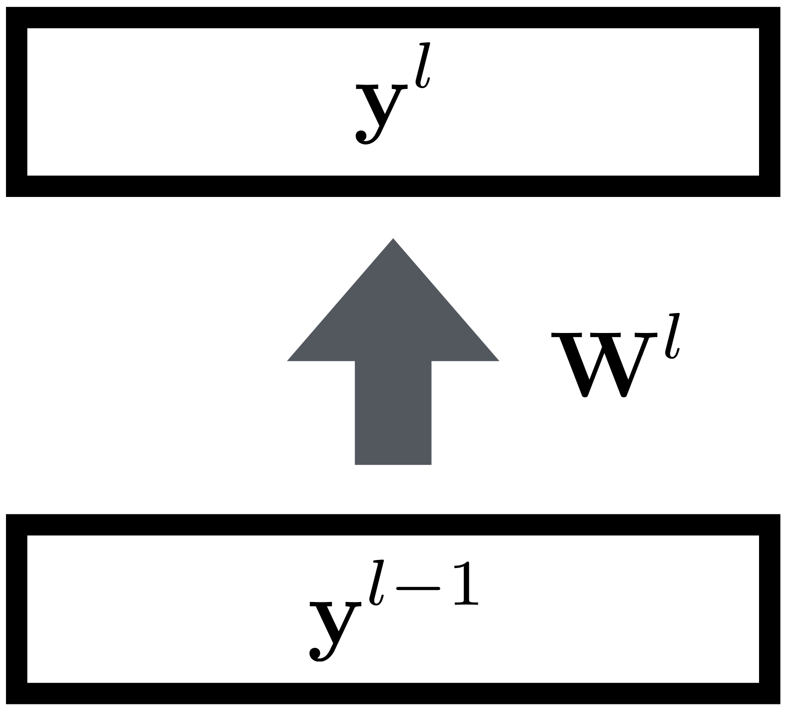

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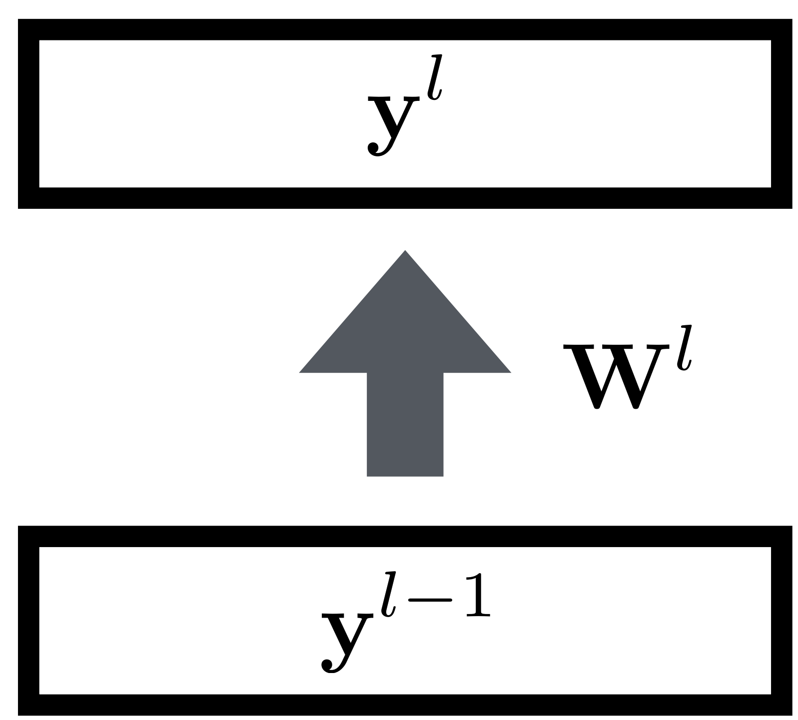
- **Single layer:** linear transformation, pointwise nonlinearity

$$\mathbf{y}^l = \sigma\left(\mathbf{W}^l \mathbf{y}^{l-1}\right)$$

$$\sigma(u) \equiv \text{leaky ReLU}$$

$$= \begin{cases} u & u \geq 0 \\ 0.05u & u < 0 \end{cases}$$



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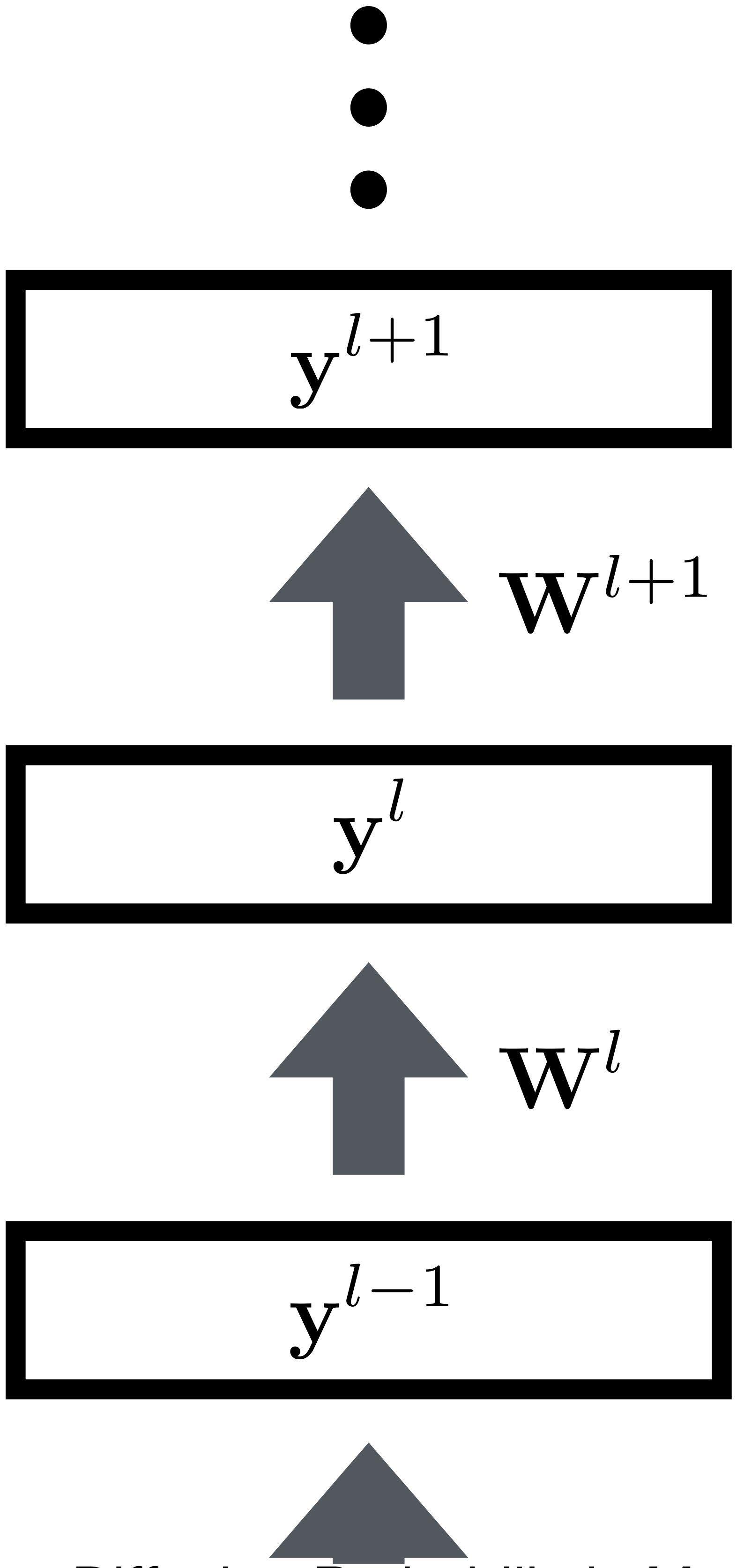

Deep Networks

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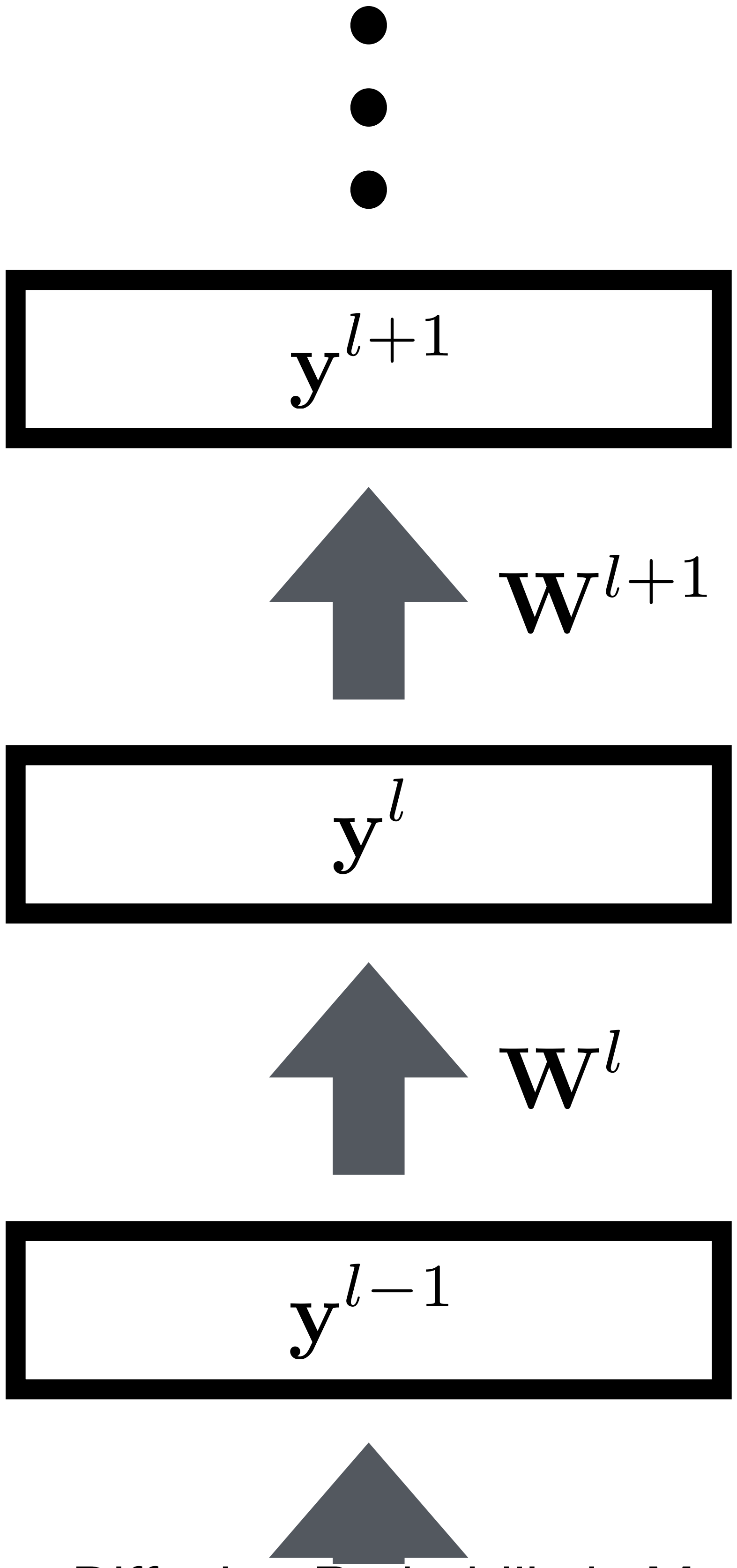
- **Single layer:** linear transformation, pointwise nonlinearity
- **Deep network:** stack single layers

$$\mathbf{y}^L = \sigma\left(\mathbf{W}^L \sigma\left(\mathbf{W}^{L-1} \cdots \sigma\left(\mathbf{W}^1 \mathbf{y}^0\right)\right)\right)$$



Convolutional Neural Network

- Single convolutional layer:
  - Same linear transform for every pixel
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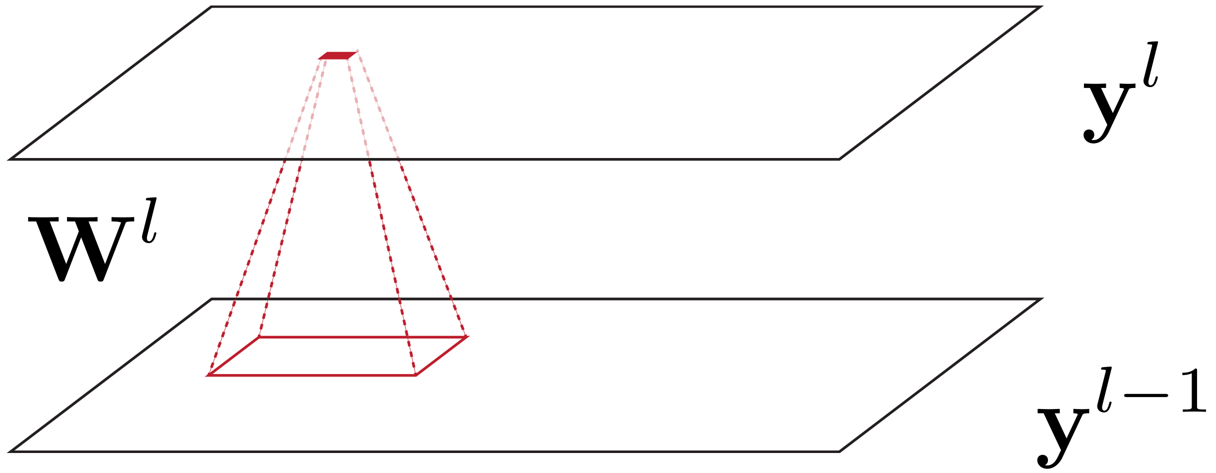
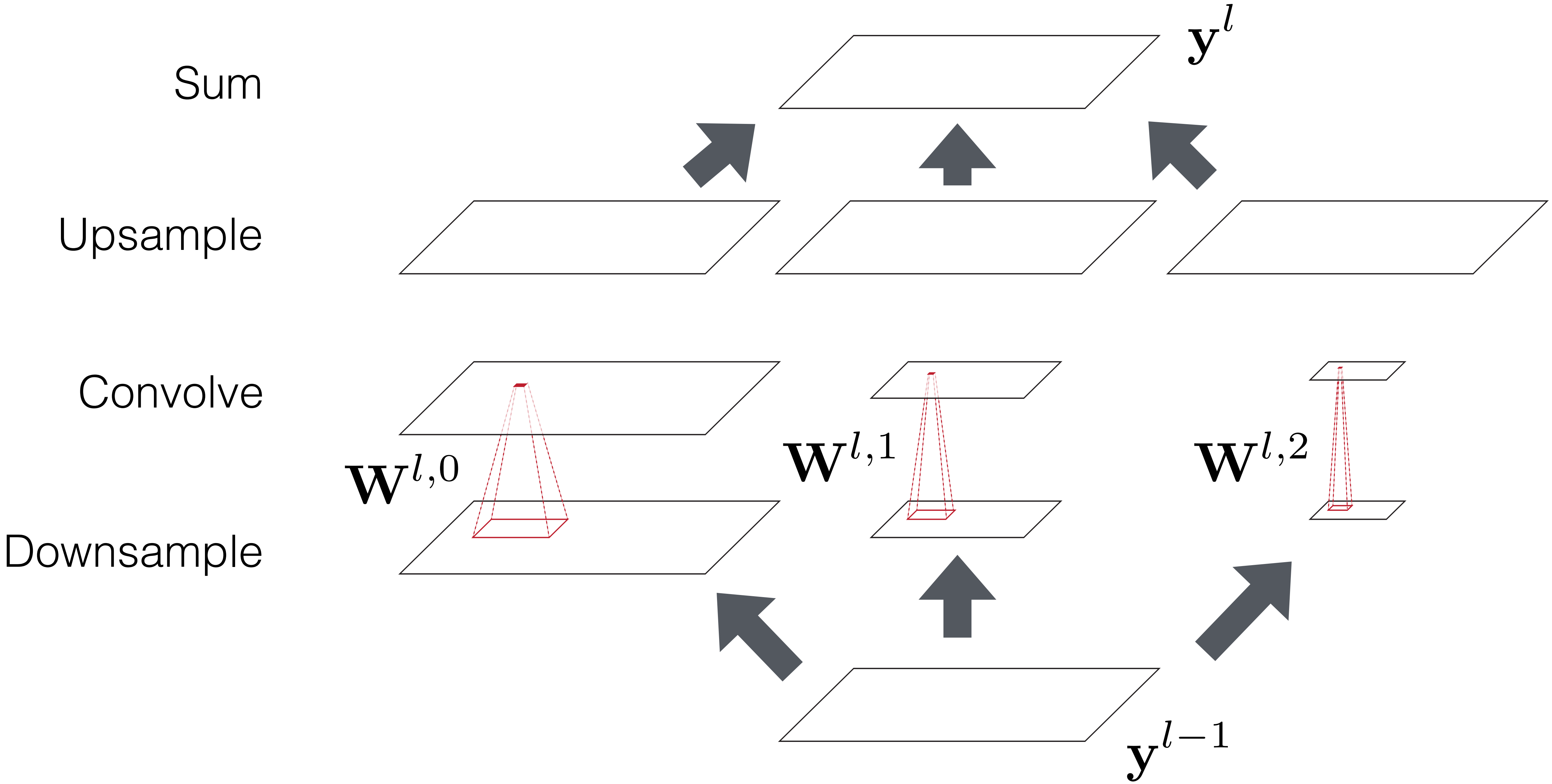


Multiscale Convolution

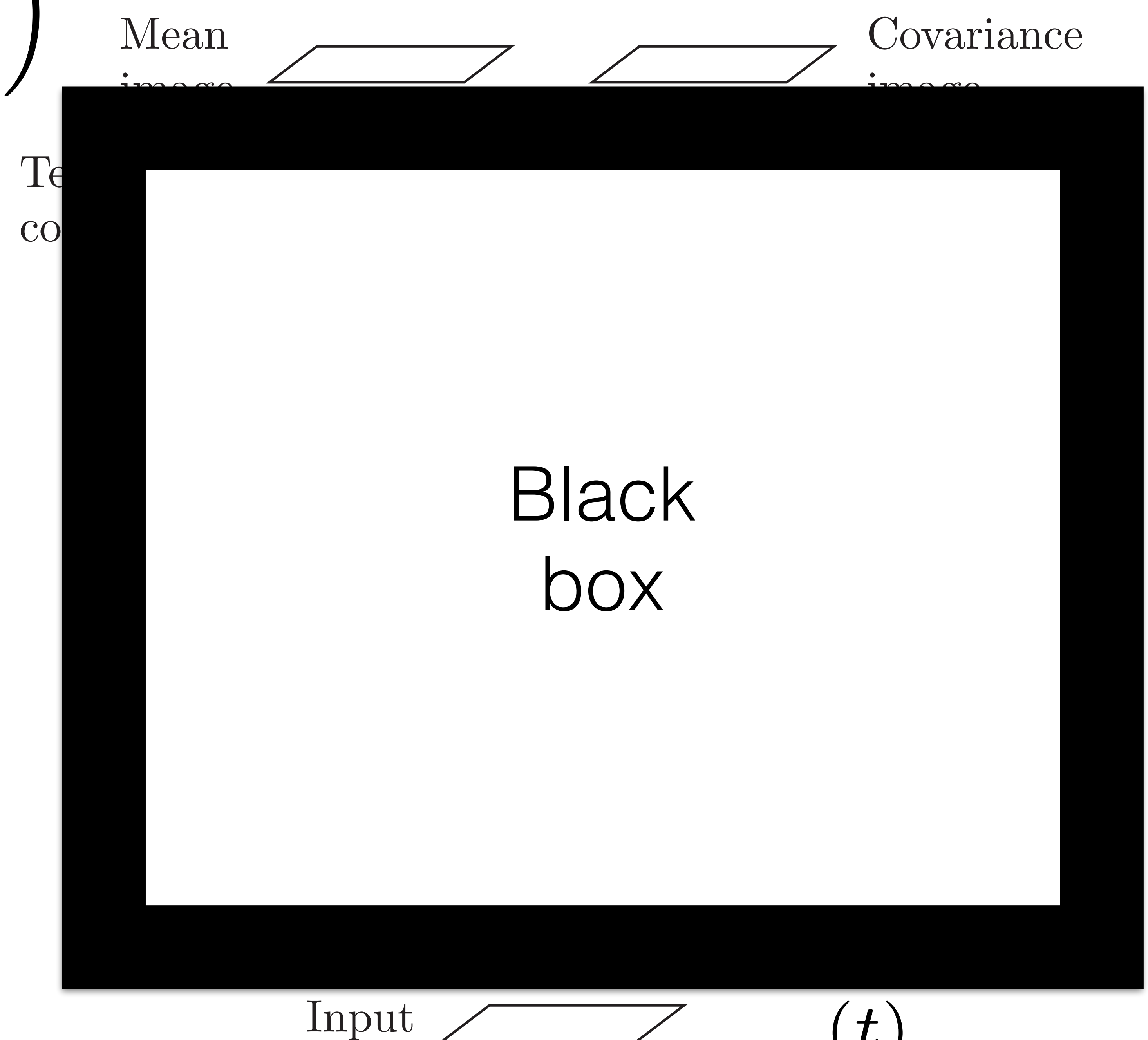
- Single multi-scale convolutional layer:



Deep Network Architecture for Diffusion

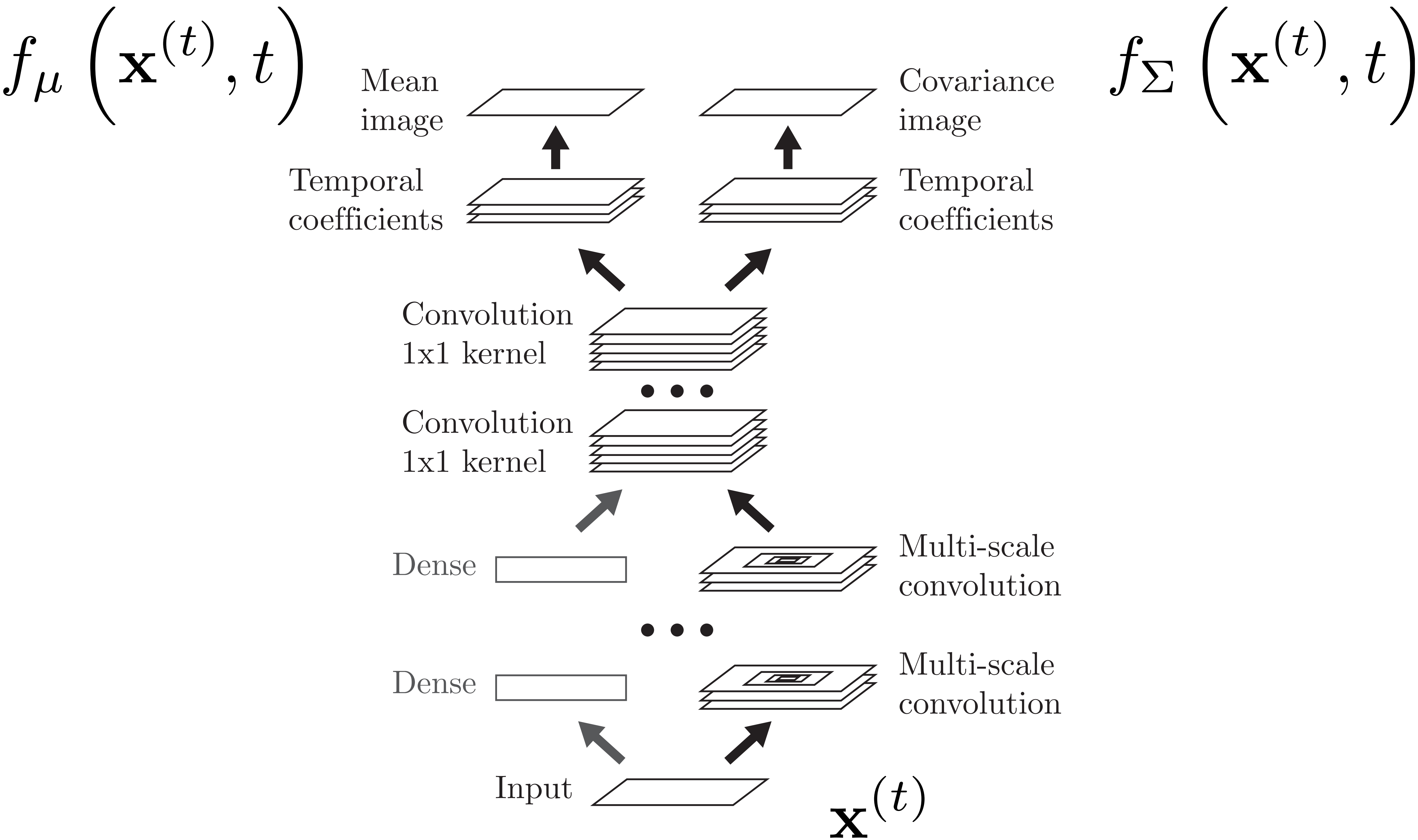
$$f_\mu\left(\mathbf{x}^{(t)}, t\right)$$

$$f_\Sigma\left(\mathbf{x}^{(t)}, t\right)$$

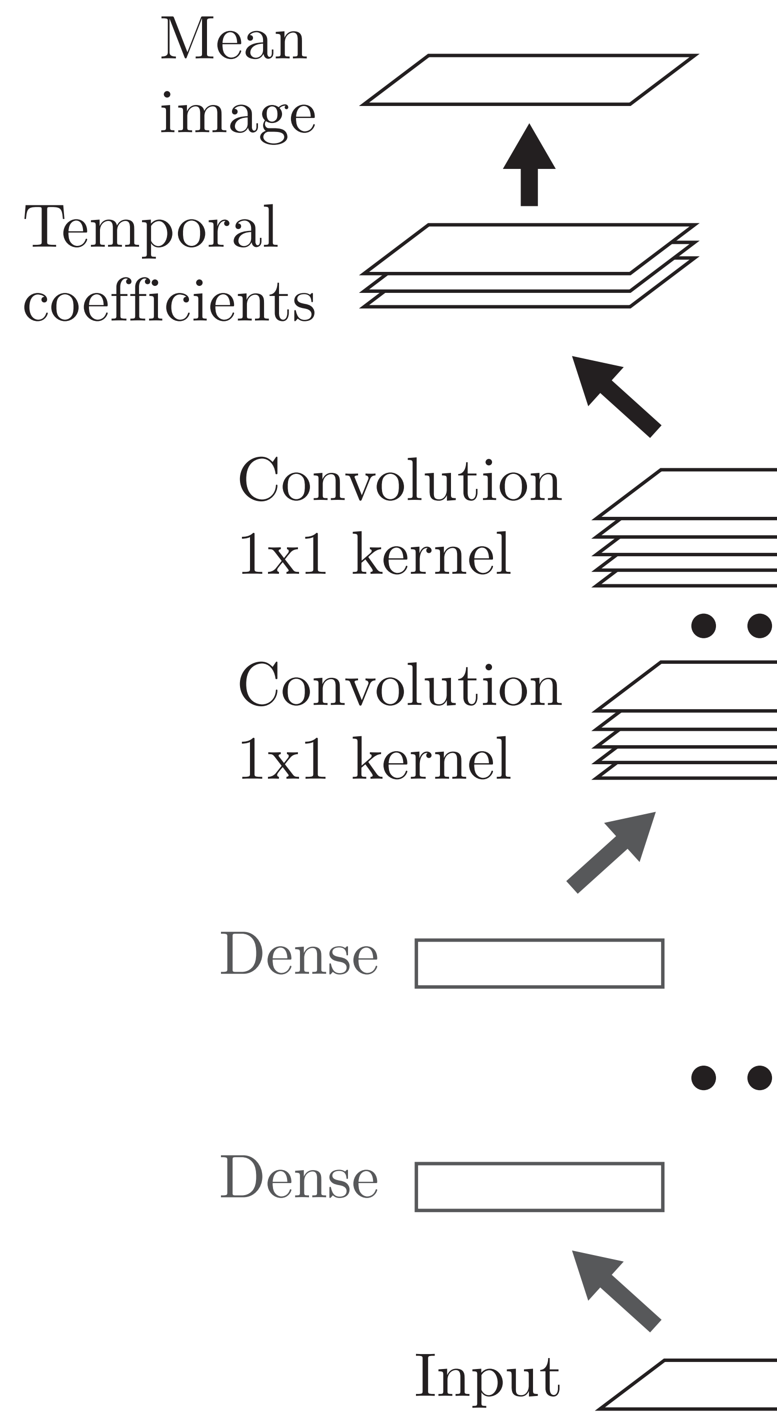


$$\mathbf{x}^{(t)}$$

Deep Network Architecture for Diffusion



Time Dependence using Temporal Basis



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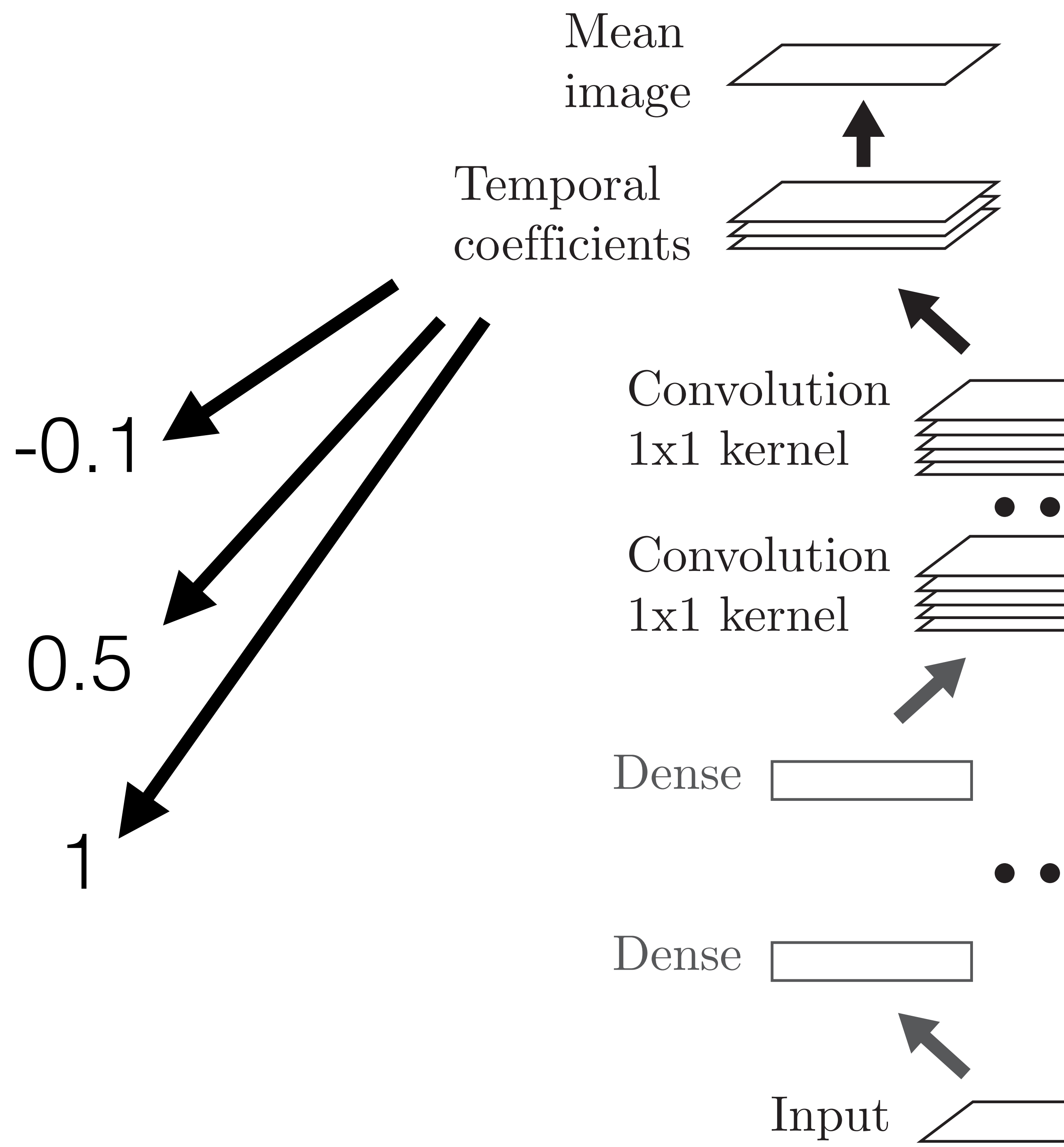

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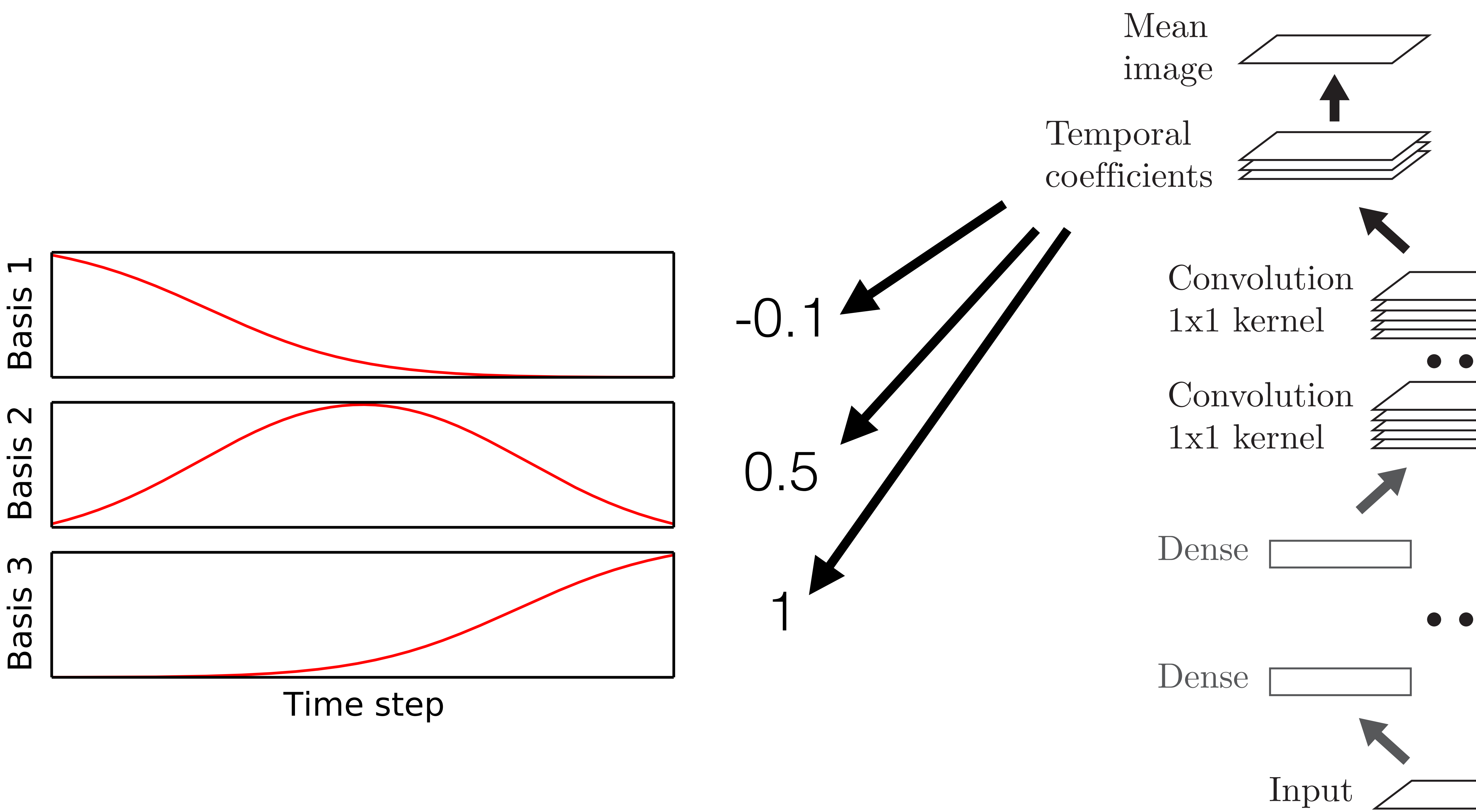
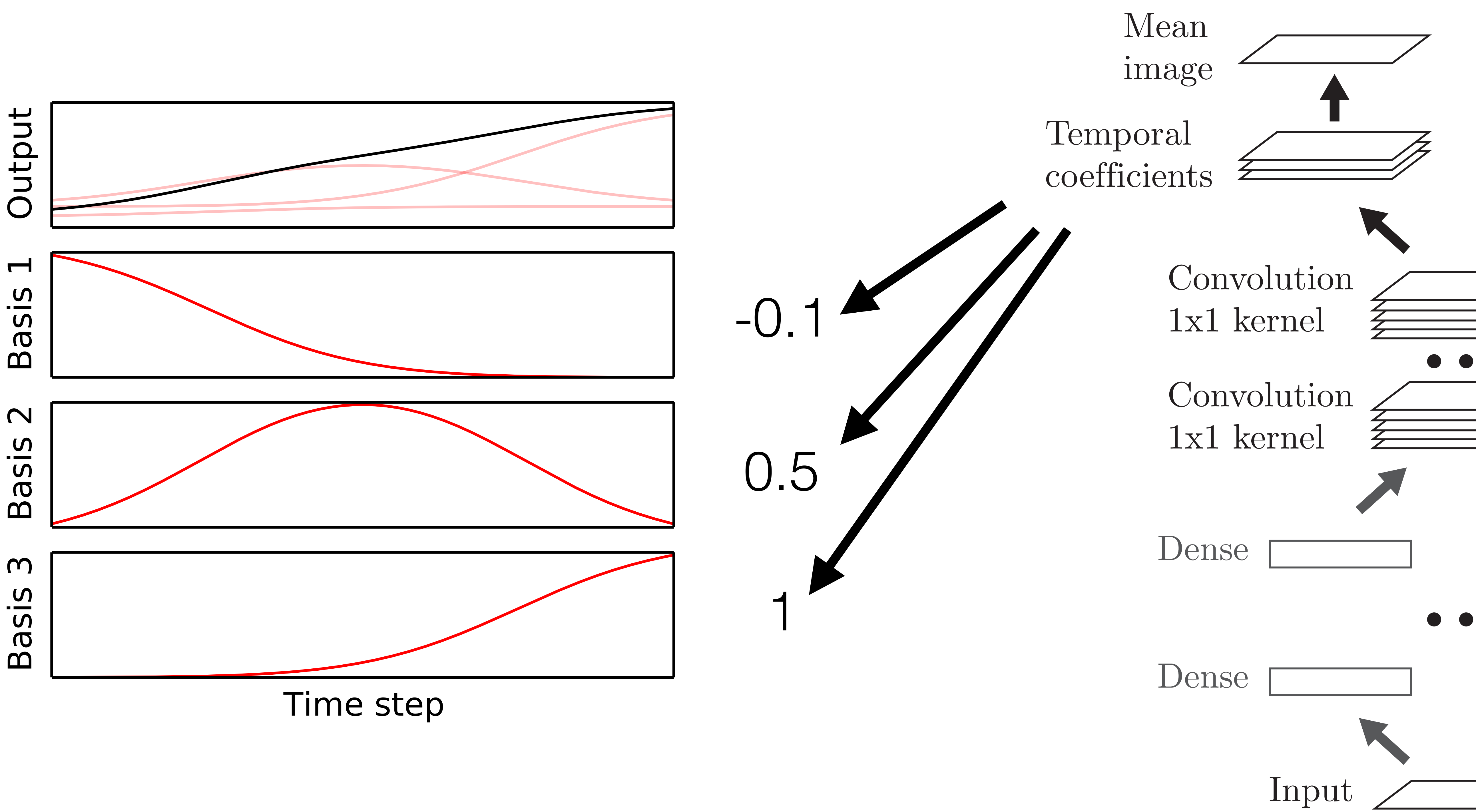
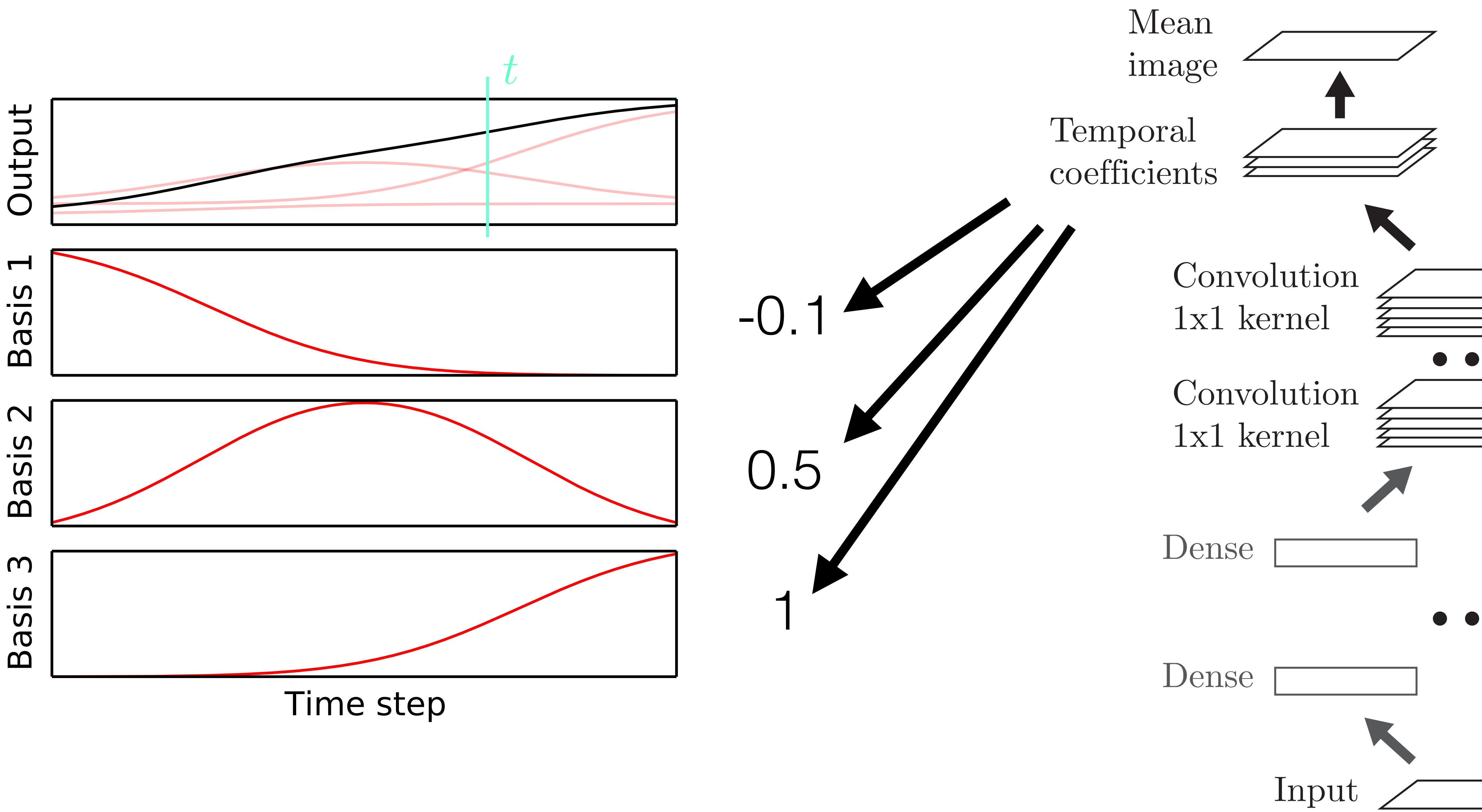


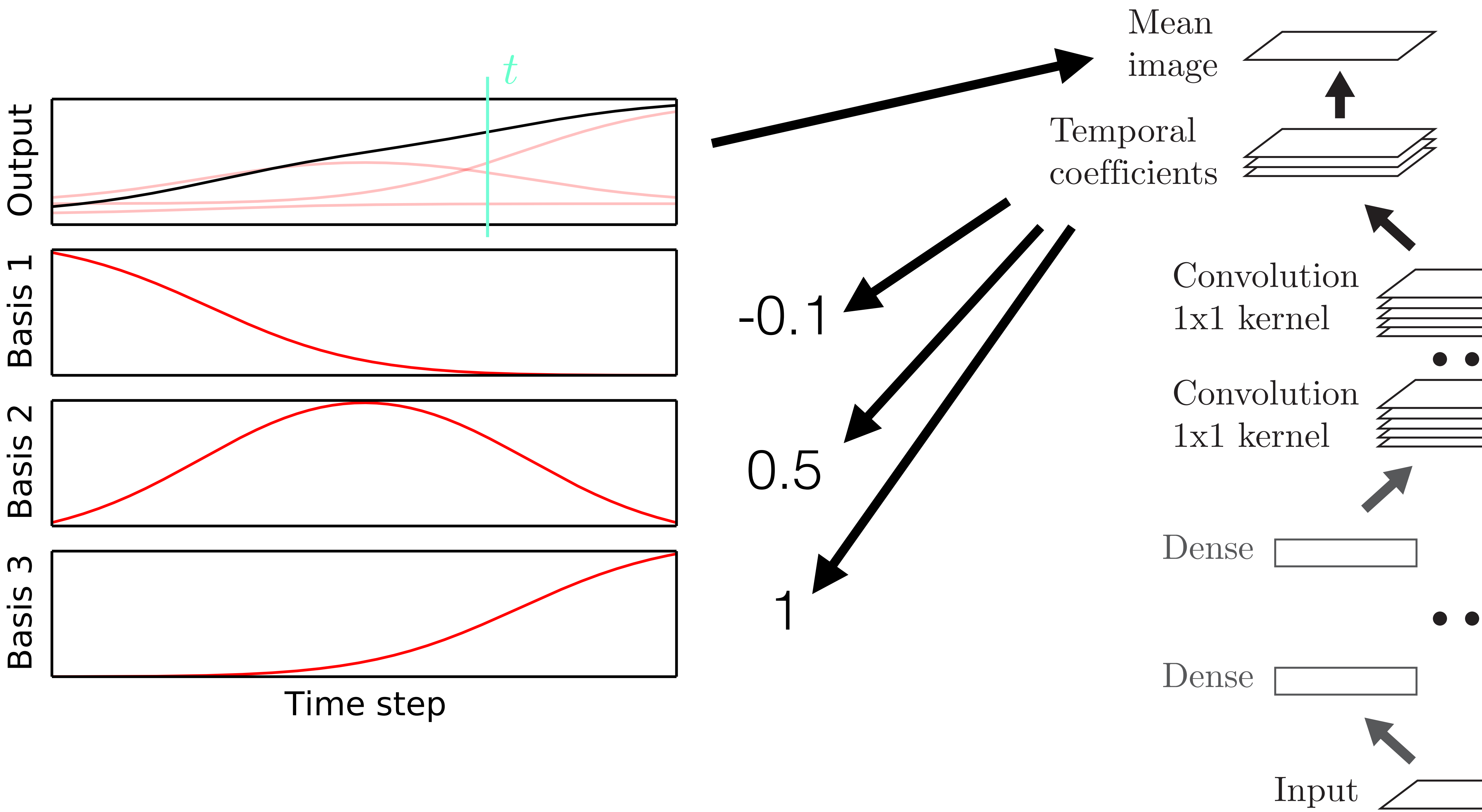
Time Dependence using Temporal Basis



Time Dependence using Temporal Basis



Time Dependence using Temporal Basis



Setting Diffusion Rate

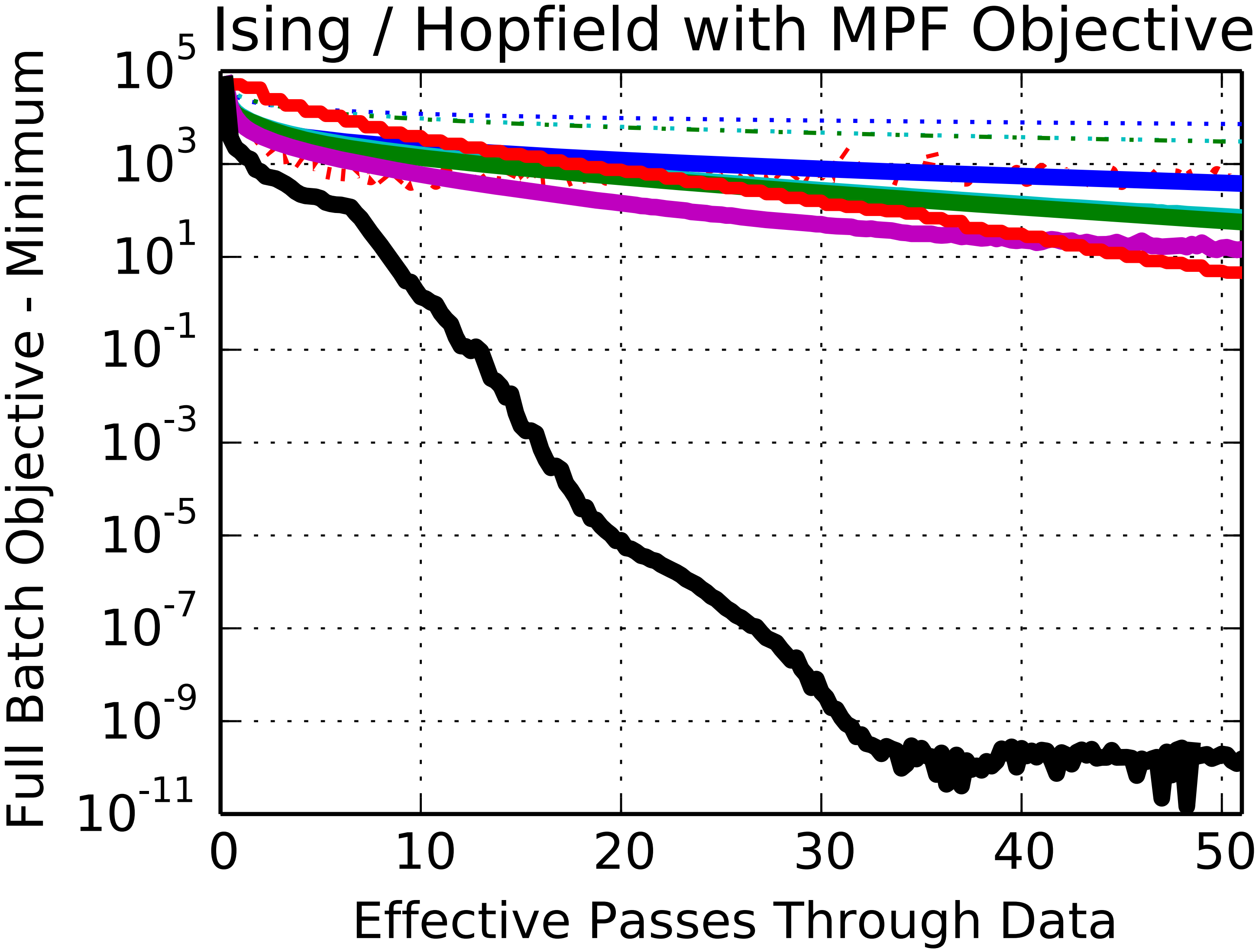
- Erase constant fraction of stimulus variance each step

$$\beta_t = \frac{1}{T - t + 1}$$

- Can also train β_t

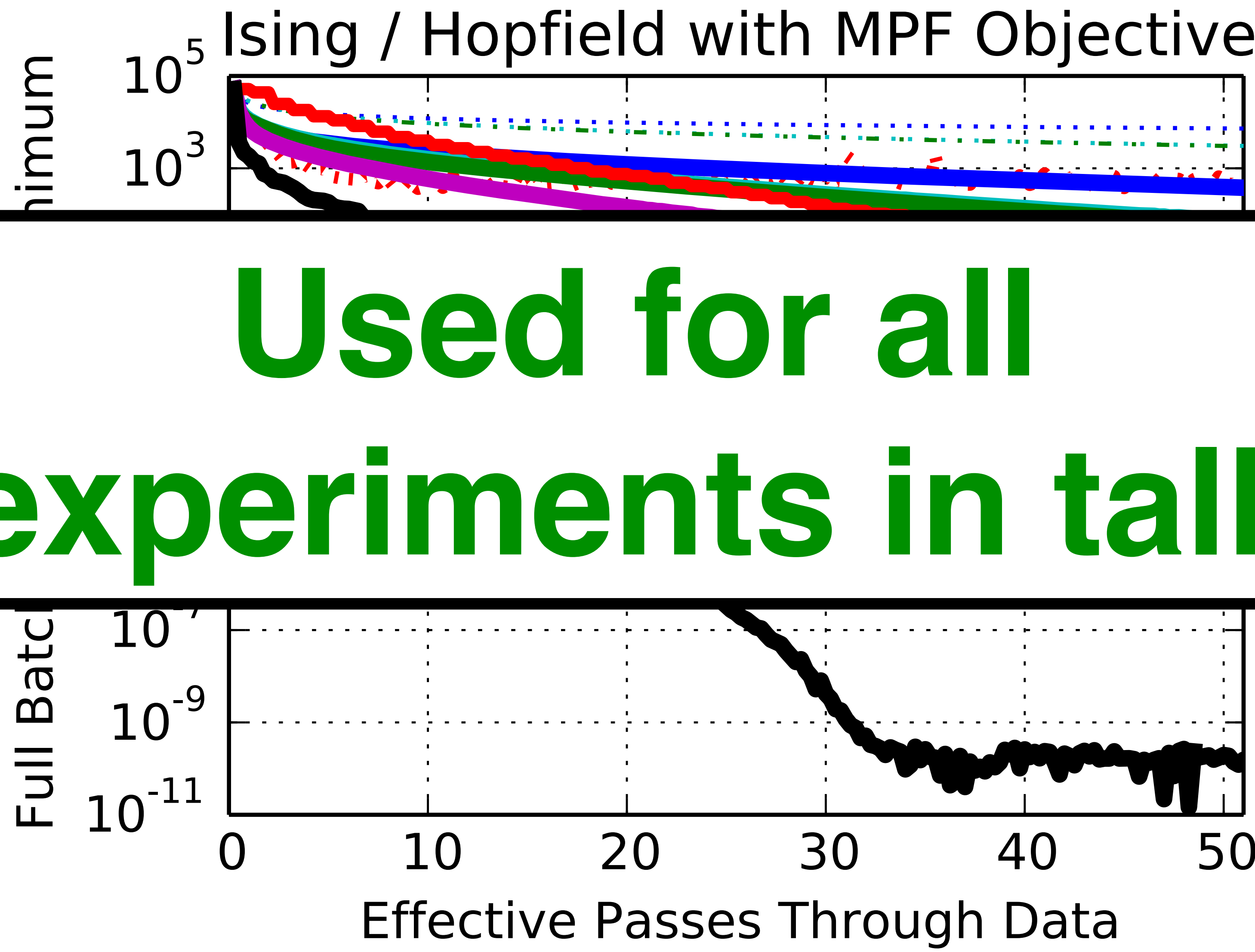
Theoretical Breakthroughs in Machine Learning

- Optimization: Combining SGD and quasi-Newton optimization (SFO optimizer) **[ICML 2014]**



Theoretical Breakthroughs in Machine Learning

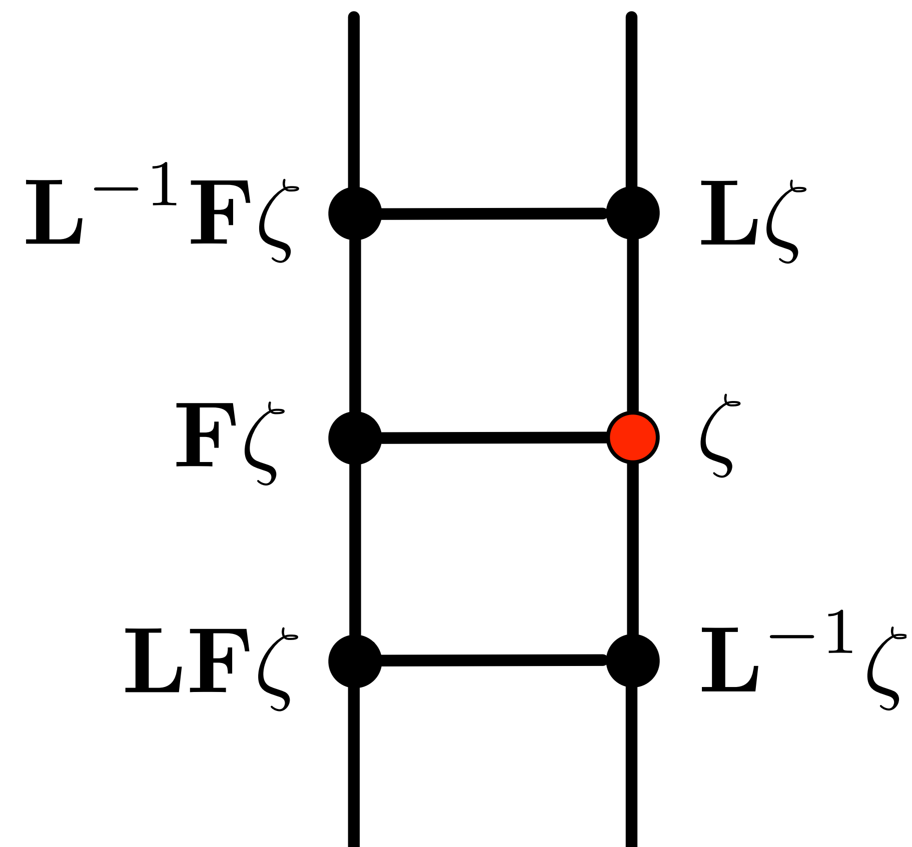
- Optimization: Combining SGD and quasi-Newton optimization (SFO optimizer) **[ICML 2014]**



Used for all experiments in talk

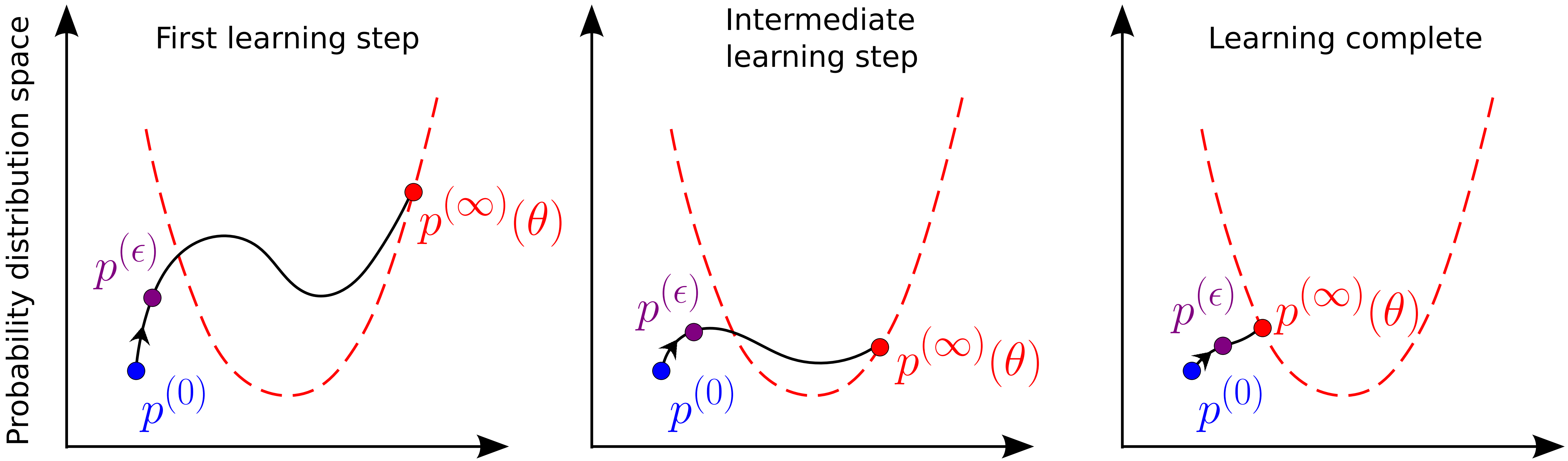
Theoretical Breakthroughs in Machine Learning

- Sampling and evaluation: Hamiltonian Monte Carlo without detailed balance **[ICML 2014]** and for log likelihood evaluation **[Tech Report 2012]**, fast sampling for natural image models **[NIPS 2012]**



Theoretical Breakthroughs in Machine Learning

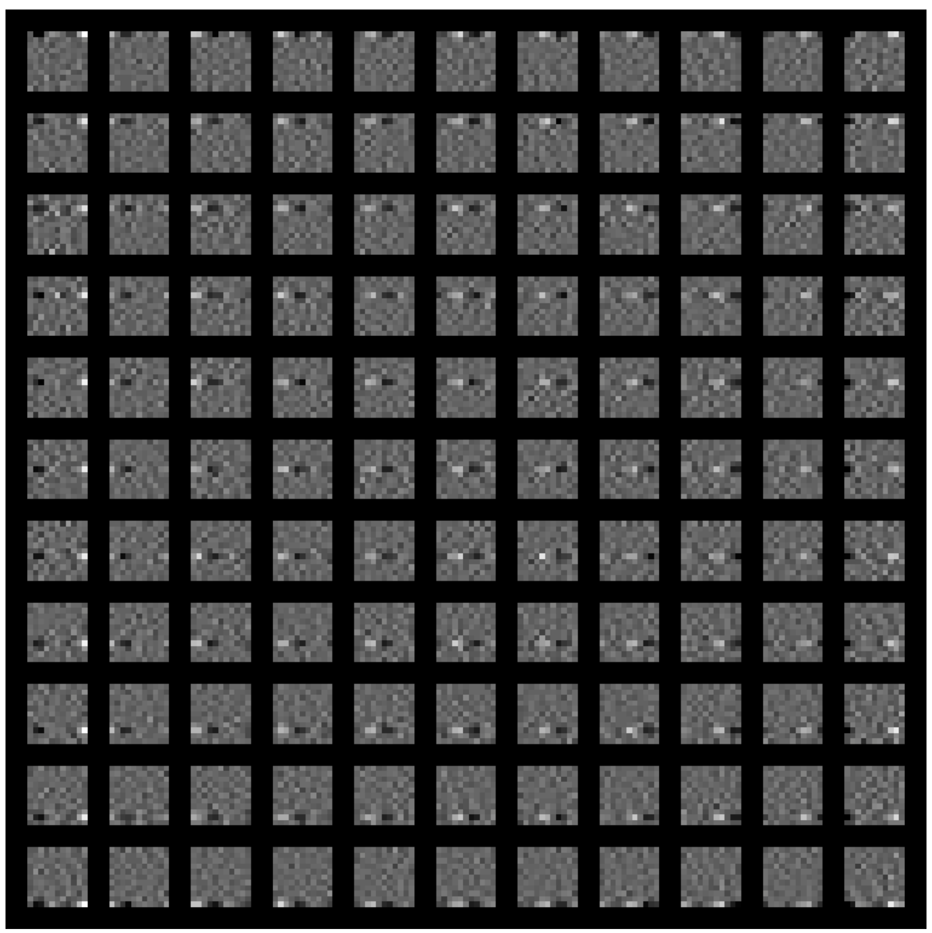
- Training energy-based models: Minimum Probability Flow learning **[ICML 2011] [PRL 2011]**

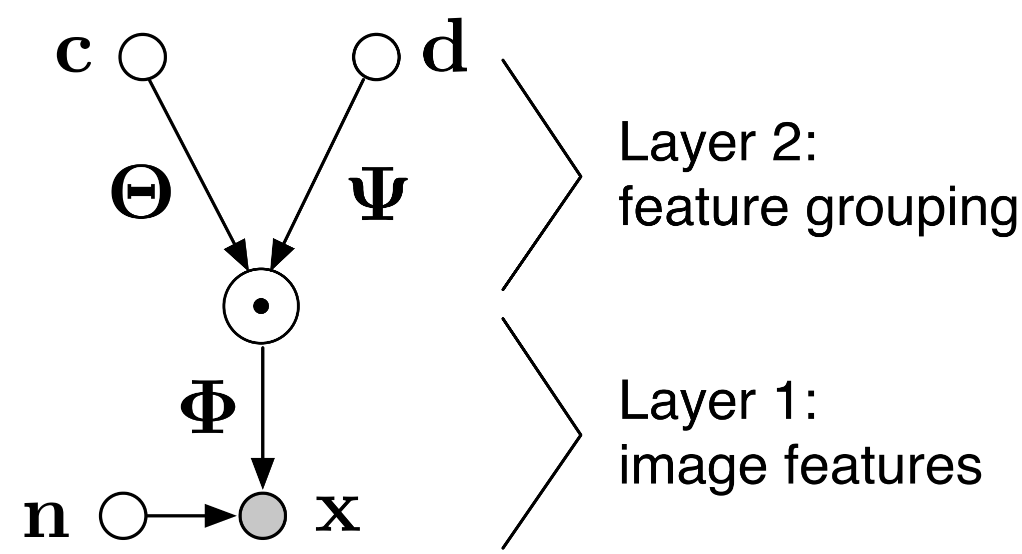


Theoretical Breakthroughs in Machine Learning

- Model design: capturing dynamics with Lie groups **[Under Revision at NECO]** , bilinear generative models **[ICCV 2011]**

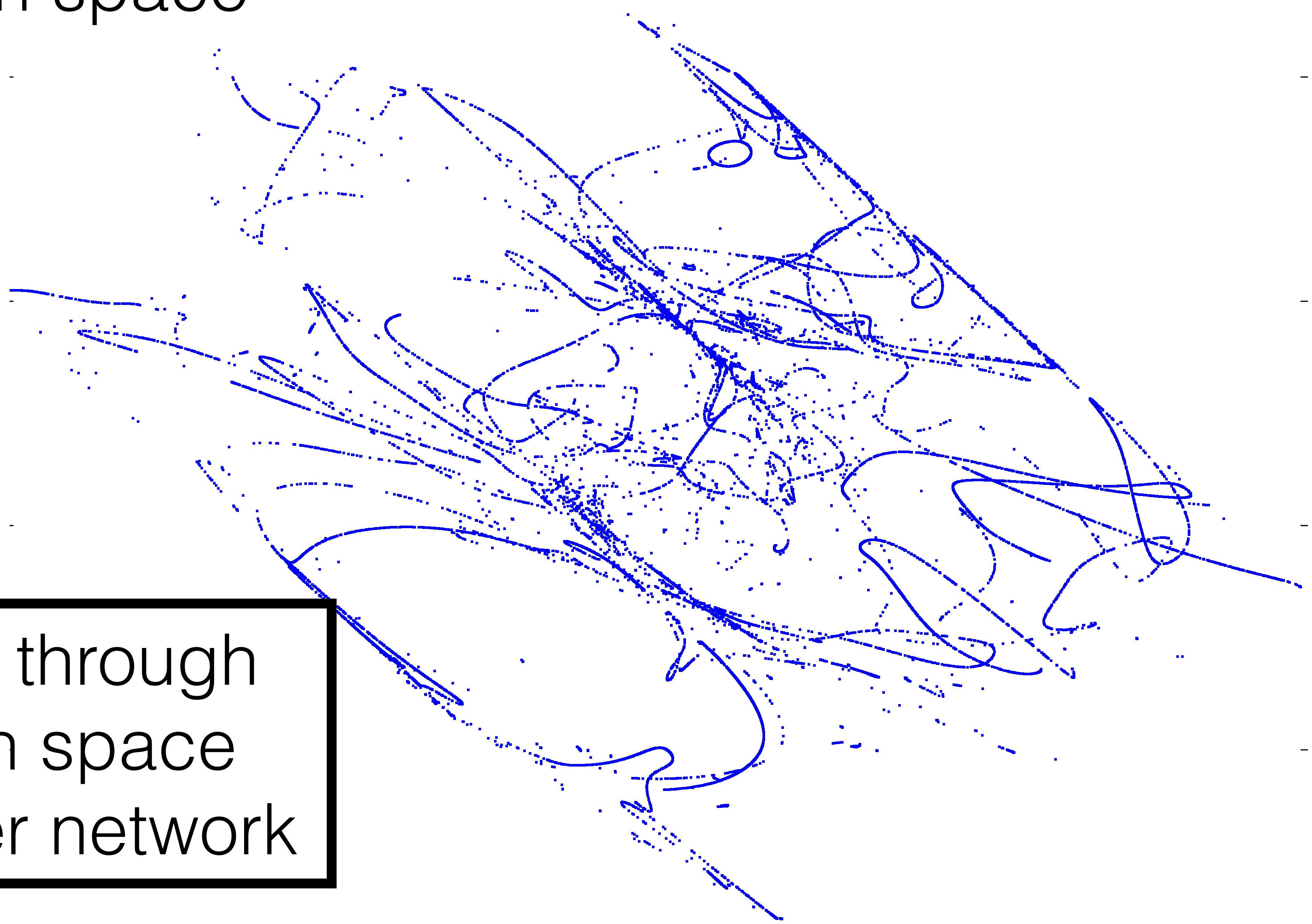
Horizontal Translation





Theoretical Breakthroughs in Machine Learning

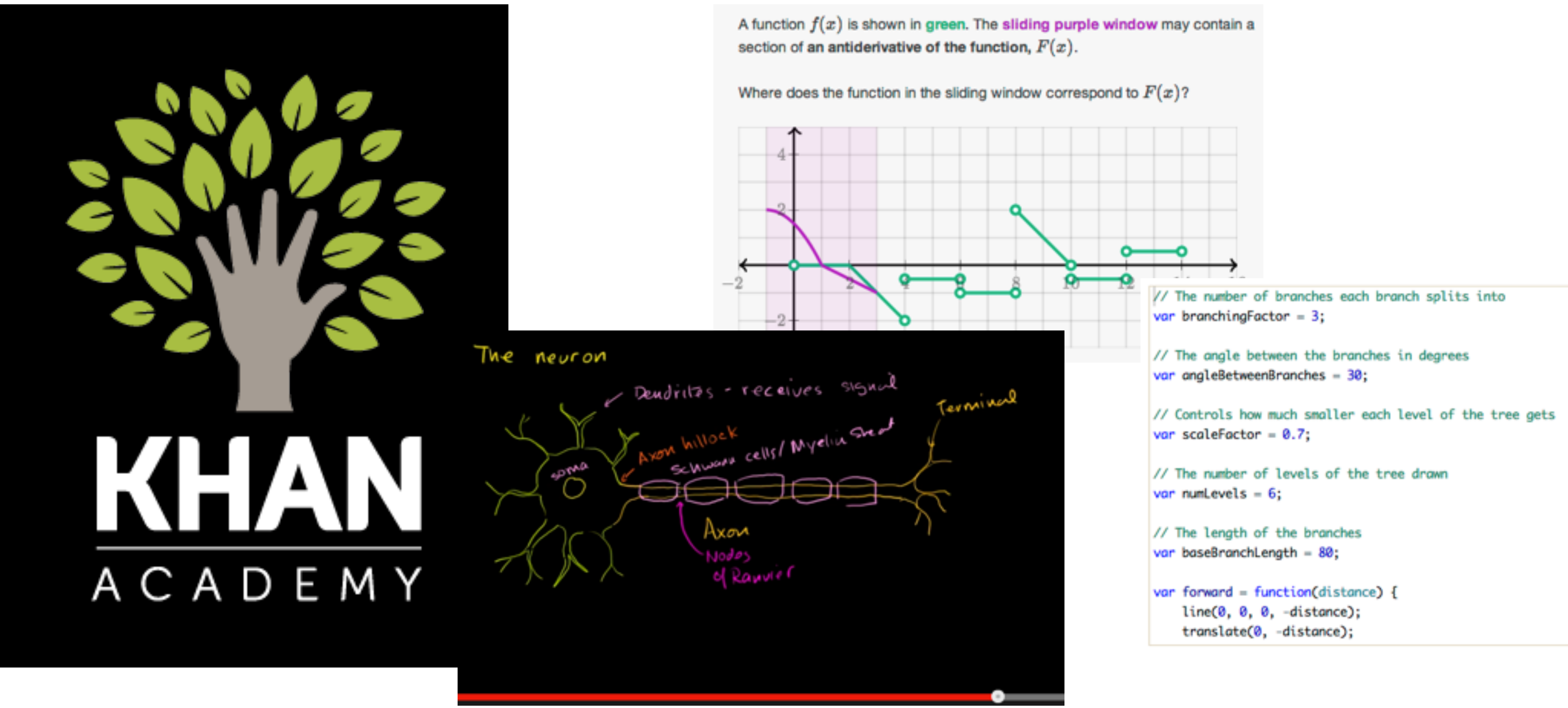
- Properties of deep networks: Characterization in function space



2d slice through function space for 2-layer network

Understanding Real Data

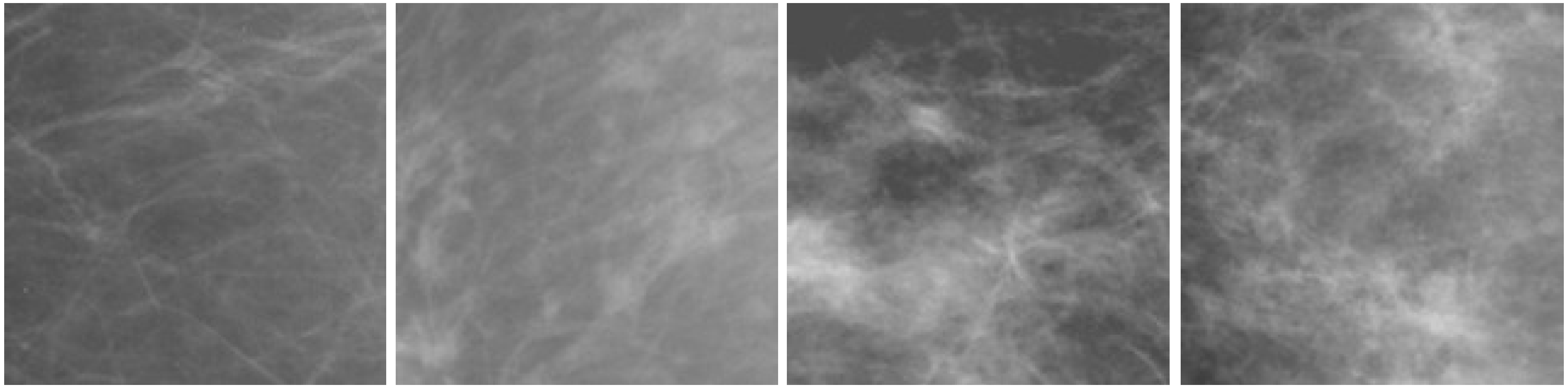
- Online education data



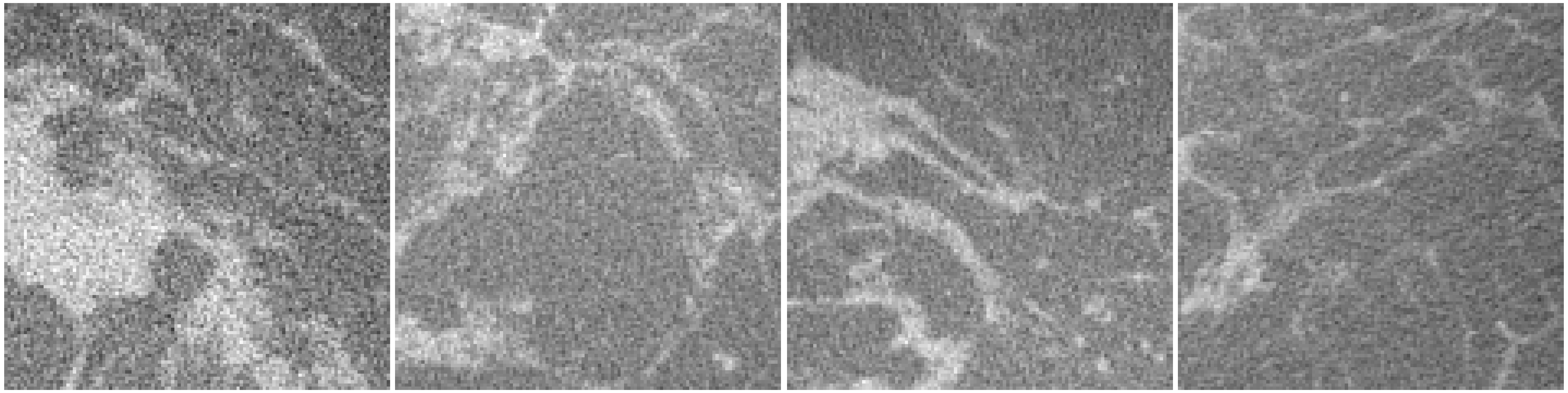
Understanding Real Data

- Medical imaging data **[SPIE 2009] [Med Phys 2014]**

A. Projection Mammograms



B. Coronal Breast CT

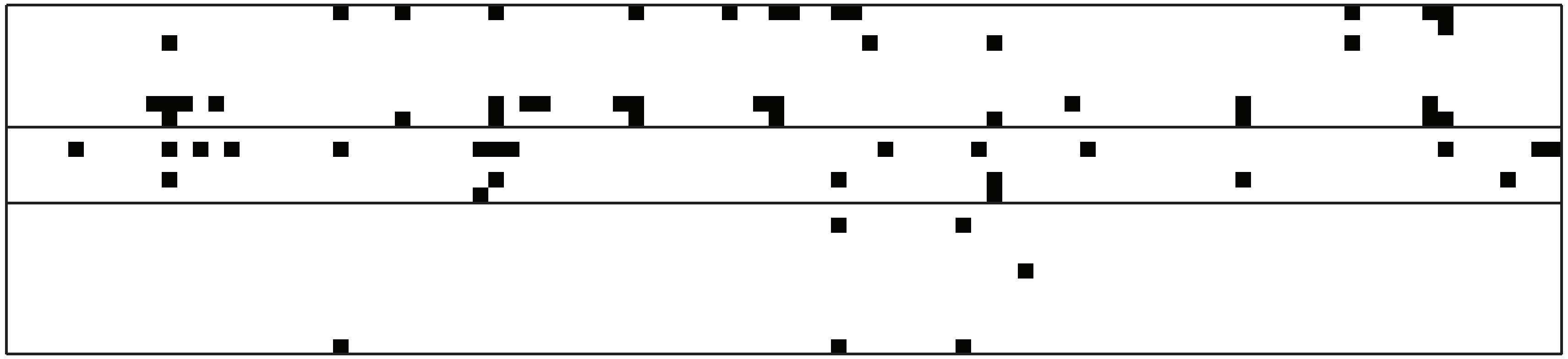


Understanding Real Data

- Neuroscience electrophysiology data: **[PLoS Comp Bio 2014] [Neuron 2013]**

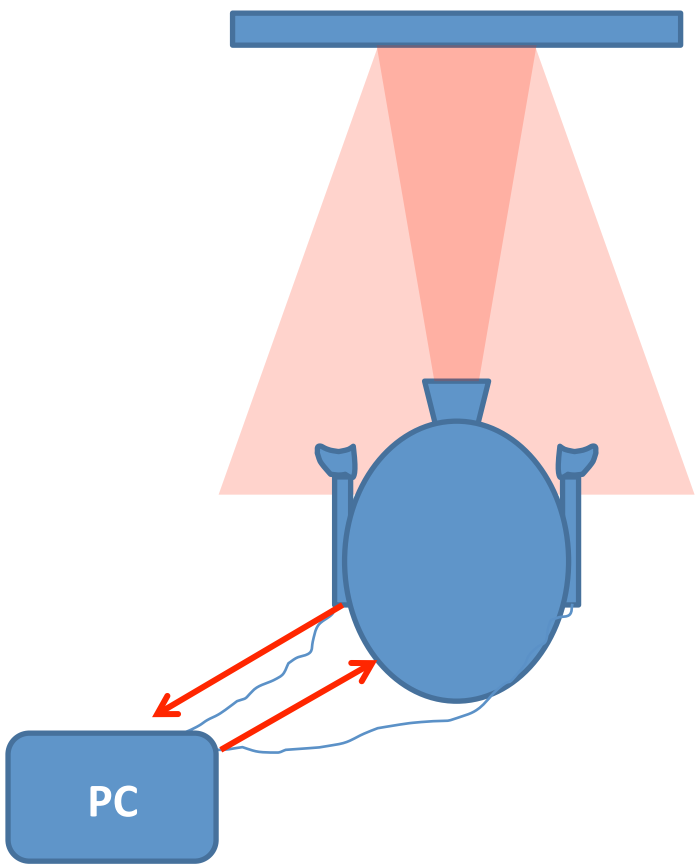
a) Stimulus frames

b) Example data, 2s of data in 20ms bins



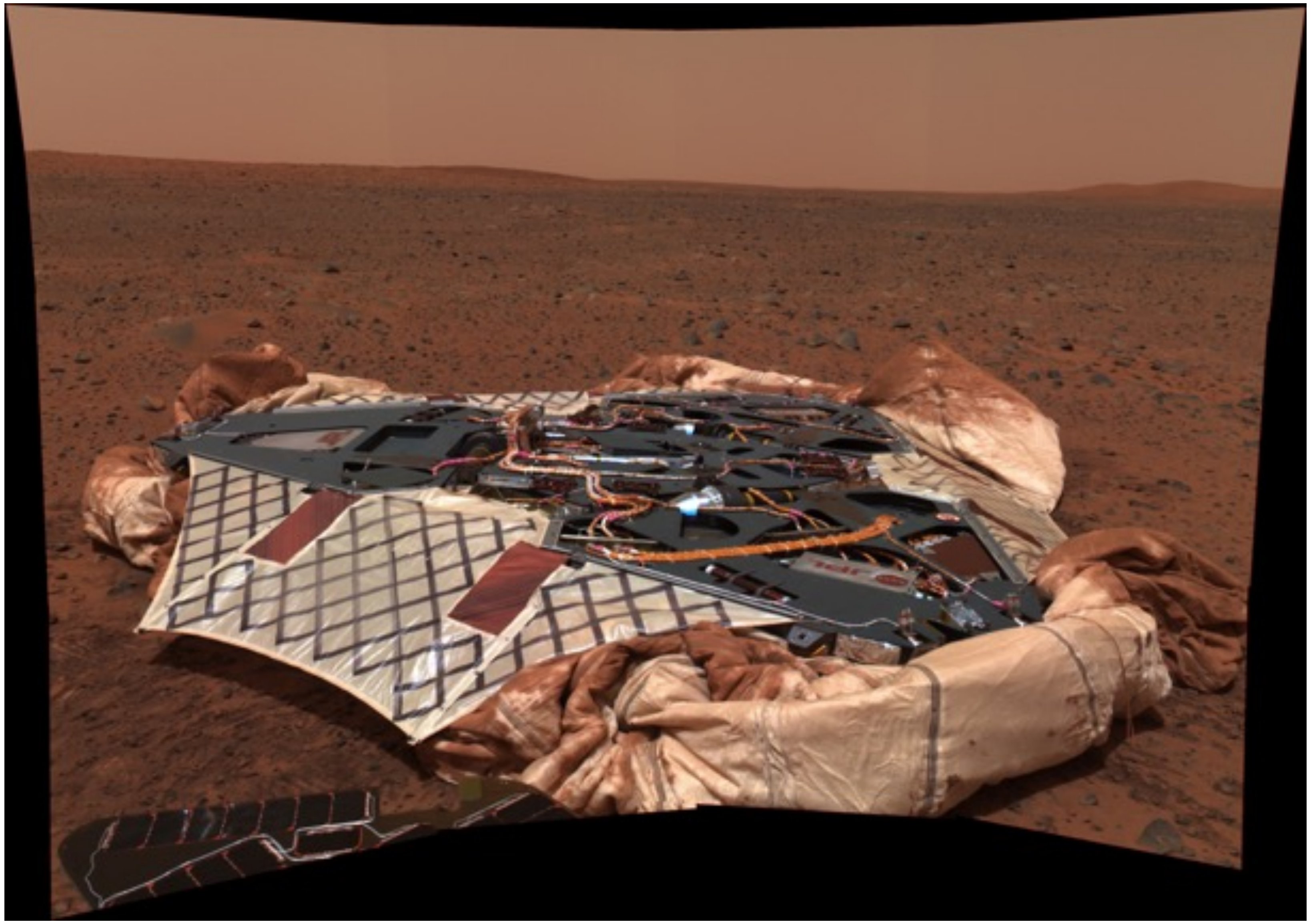
Understanding Real Data

- Human ultrasonic echolocation: Blind assistive device
  [TBME 2015]



Understanding Real Data

- Planetary science: multispectral observations
  [Science 2004a] [Science 2004b]



Thanks!

Collaborators

- Craig Abbey
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- Jack Culpepper
- Liberty Hamilton
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- Alex Huth
- Kilian Koepsell
- Urs Köster
- Niru Maheswaranathan
- Mayur Mudigonda
- Ben Poole
- Lucas Theis
- Jimmy Wang
- Eric Weiss

Mentors

- Surya Ganguli
- Bruno Olshausen
- Michael R. DeWeese
- James F. Bell III

Endless discussion

- The Redwood Center for Theoretical Neuroscience
- The Ganguli Gang

Eric Weiss

Niru Maheswaranathan

Surya Ganguli

Differences from Variational Autoencoders

- Can analytically evaluate KL divergence between steps in forward and reverse trajectories.
- Can multiply with other distributions, and compute posteriors
- Erases structure, rather than transforming it
- Thousands of layers or time steps, rather than only a small handful
- Connections to nonequilibrium statistical mechanics

Continuous Time

$$q\left(\mathbf{x}^t|\mathbf{x}^0,\mathbf{x}^{t+dt}\right)=\mathcal{N}\left(\mathbf{x}^t;\mathbf{x}^{t+dt}-\mathbf{x}^{t+dt}\frac{\exp\left(-\beta t\right)}{1-\exp\left(-\beta t\right)}\beta dt-\frac{1}{2}\mathbf{x}^{t+dt}\beta dt+\frac{1}{2}\mathbf{x}^0\operatorname{csch}\left(\frac{\beta t}{2}\right)\beta dt,\beta dt\right)$$

$$p\left(\mathbf{x}^t|\mathbf{x}^{t+dt}\right)=\mathcal{N}\left(\mathbf{x}^t;\mathbf{x}^{t+dt}-\mathbf{x}^{t+dt}\frac{\exp\left(-\beta t\right)}{1-\exp\left(-\beta t\right)}\beta dt-\frac{1}{2}\mathbf{x}^{t+dt}\beta dt+\frac{1}{2}f_0\left(\mathbf{x}^{t+dt},t\right)\operatorname{csch}\left(\frac{\beta t}{2}\right)\beta dt,\beta dt\right)$$

$$\begin{aligned}D_{KL}\left(q\left(\mathbf{x}^t|\mathbf{x}^0,\mathbf{x}^{t+dt}\right)||p\left(\mathbf{x}^t|\mathbf{x}^{t+dt}\right)\right)&=\frac{1}{2}\frac{\Sigma_q}{\Sigma_p}+\frac{1}{2}\log\frac{\Sigma_p}{\Sigma_q}+\frac{1}{2}\frac{\left(\mu_p-\mu_q\right)^2}{\Sigma_p}-\frac{1}{2}\\&=\frac{1}{8}\left(f_0\left(\mathbf{x}^{t+dt},t\right)-\mathbf{x}^0\right)^2\operatorname{csch}^2\left(\frac{\beta t}{2}\right)\beta dt\end{aligned}$$

Denoising autoencoder penalty

Related Methods

- Generative stochastic networks
- Variational autoencoders
- (Deep) (Recurrent) Neural Autoregressive Distribution Estimators

- Variational Bayesian(e.g. variational autoencoder)
    - Posterior over intermediate layers has analytic form — > KL divergence has analytic form
    - Can multiply distributions
    - Generative model is small perturbation around inference model — makes learning easier
    - Models have *thousands* of layers (or time steps)