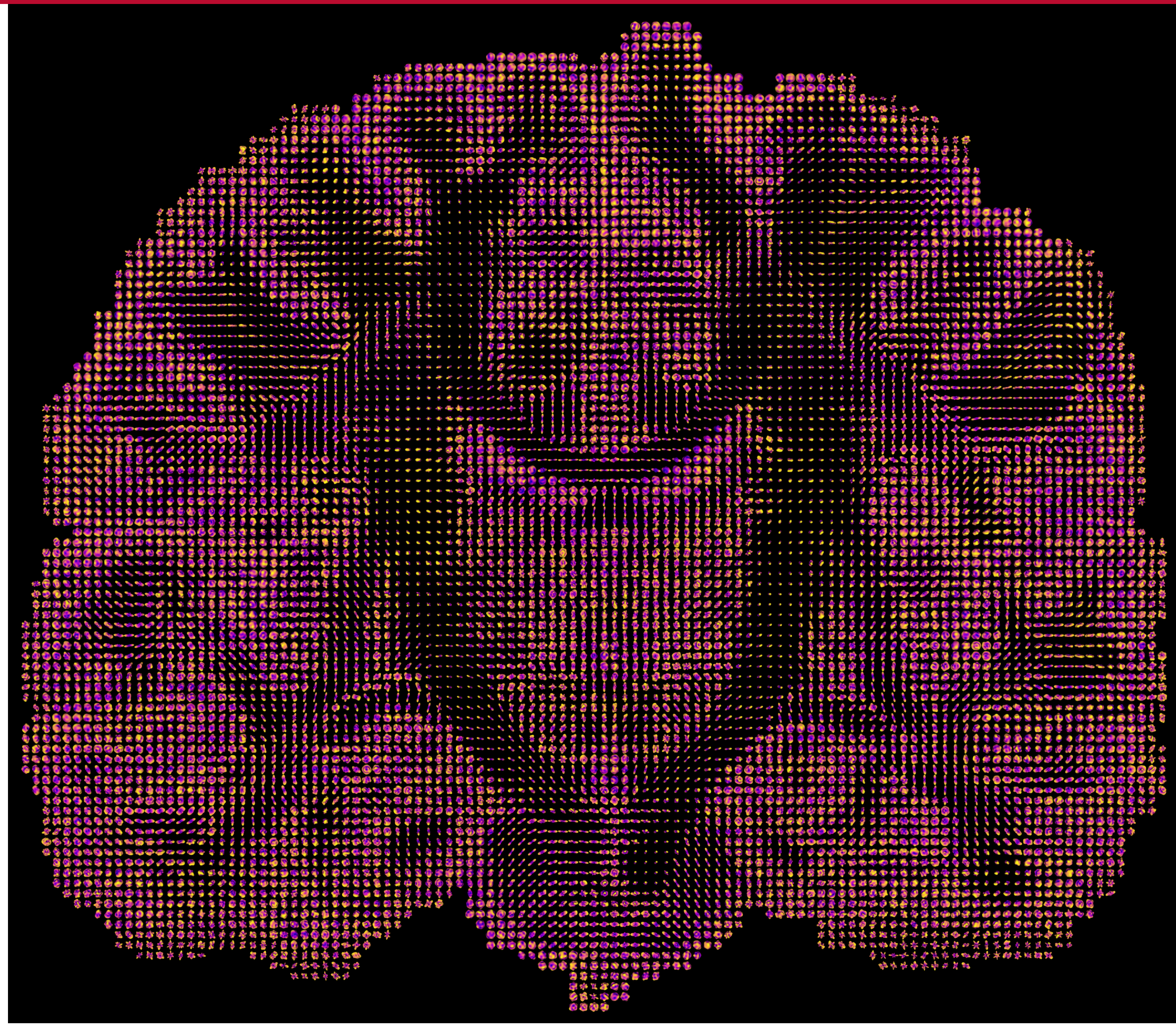
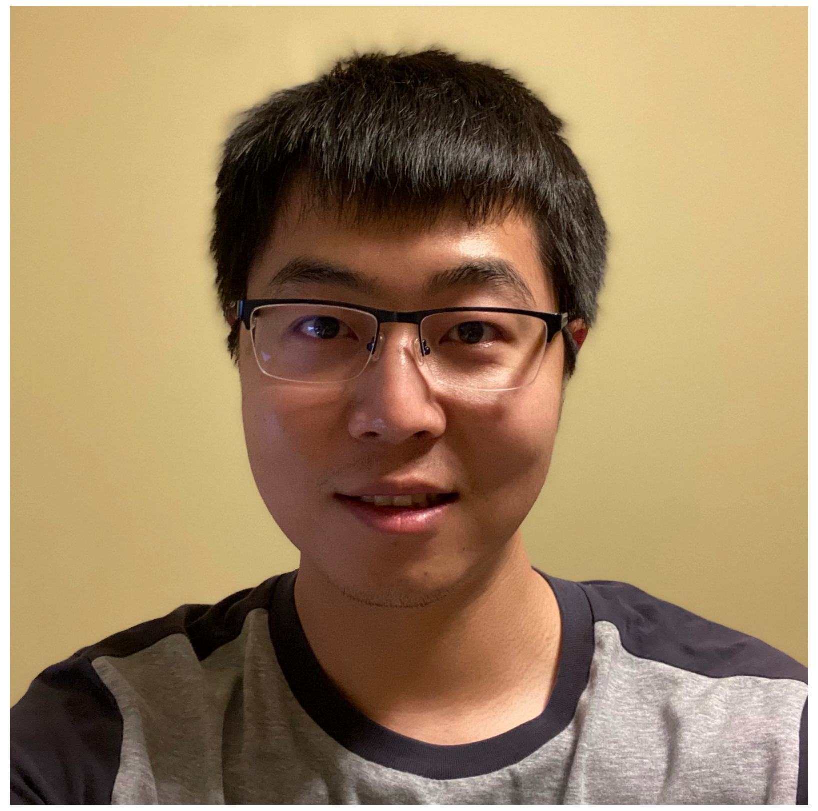
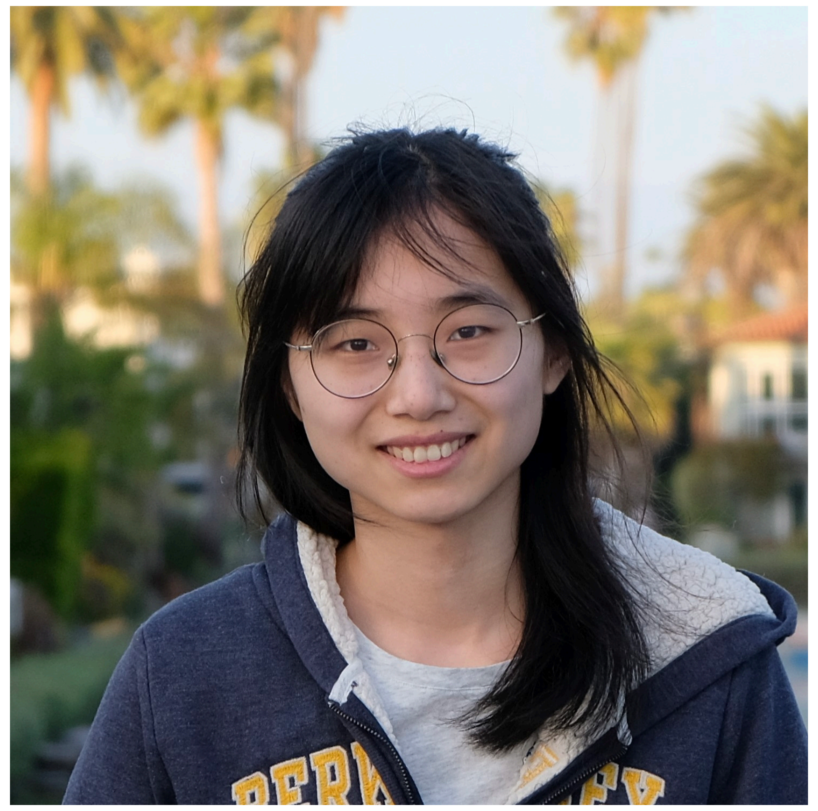
Flow-based Generative Models For Learning Manifold to Manifold Mappings



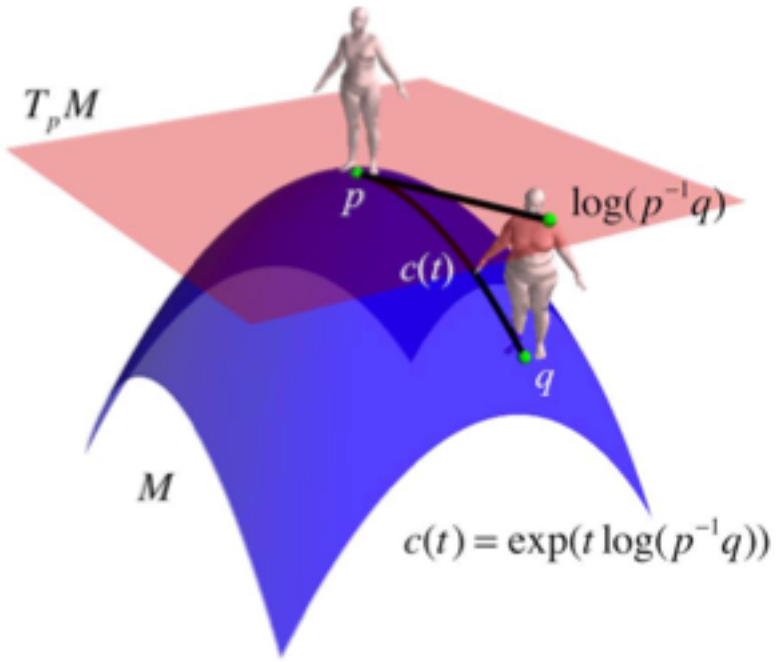
Xingjian Zhen, Rudrasis Chakraborty, Liu Yang, Vikas Singh



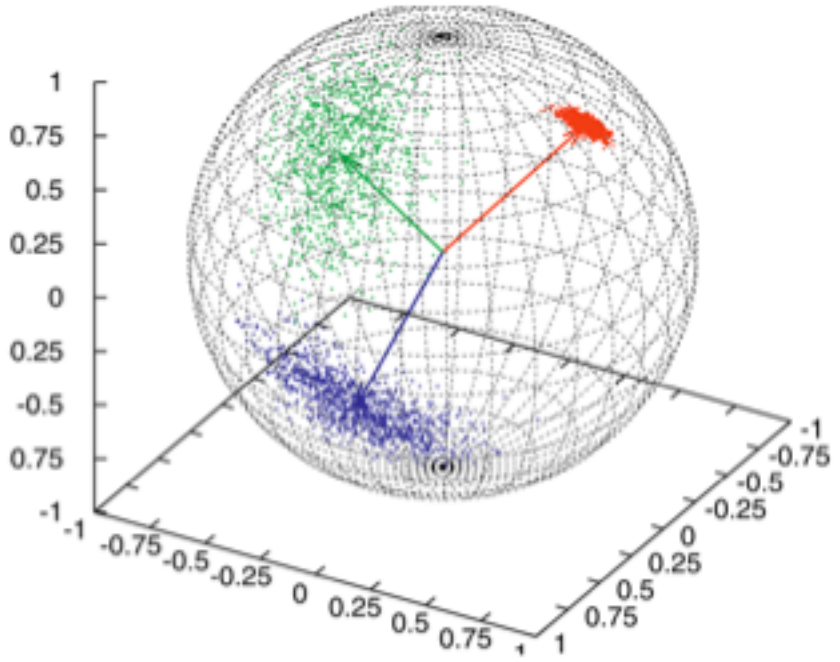


Manifold data arises in many application

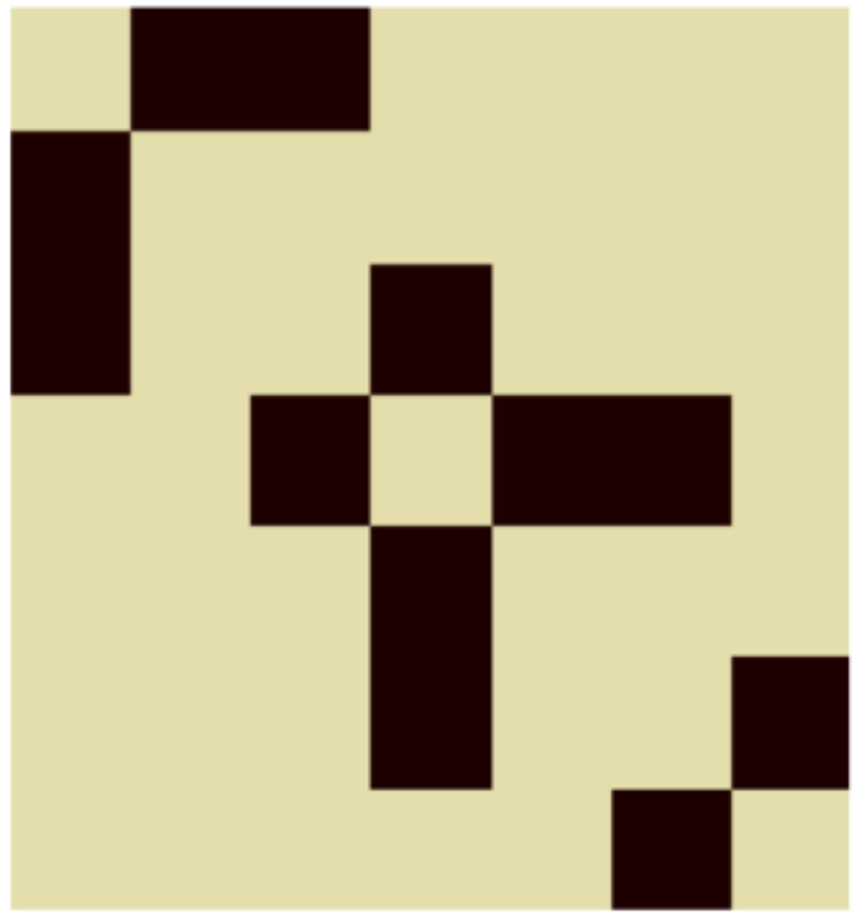
(a) Shapes



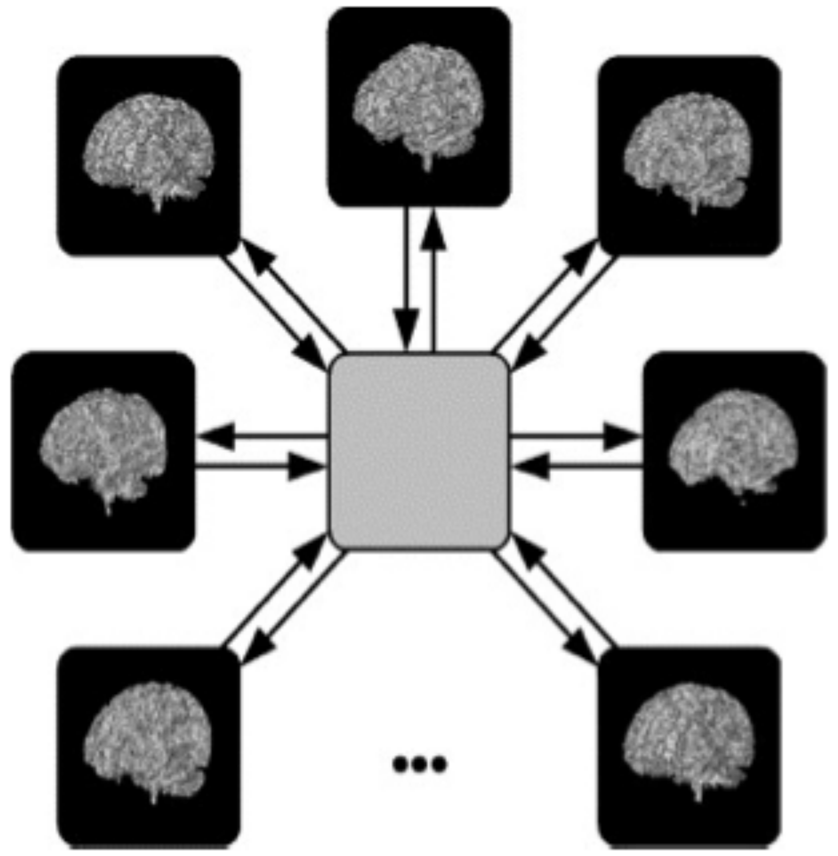
(b) Lie body manifolds



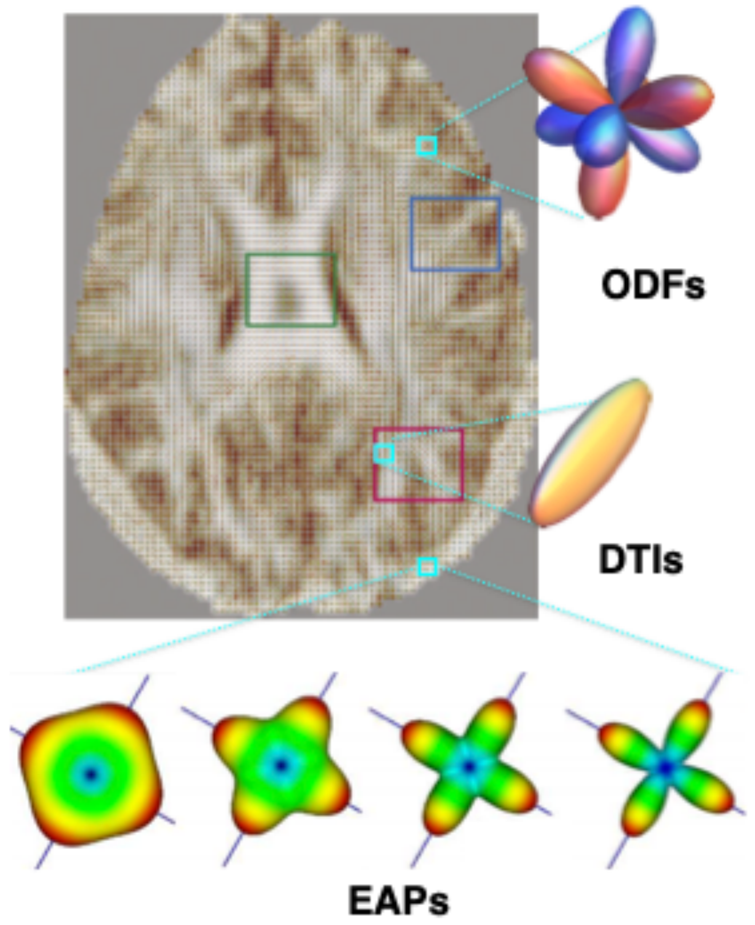
(c) Directional data



(d) Covariance matrix

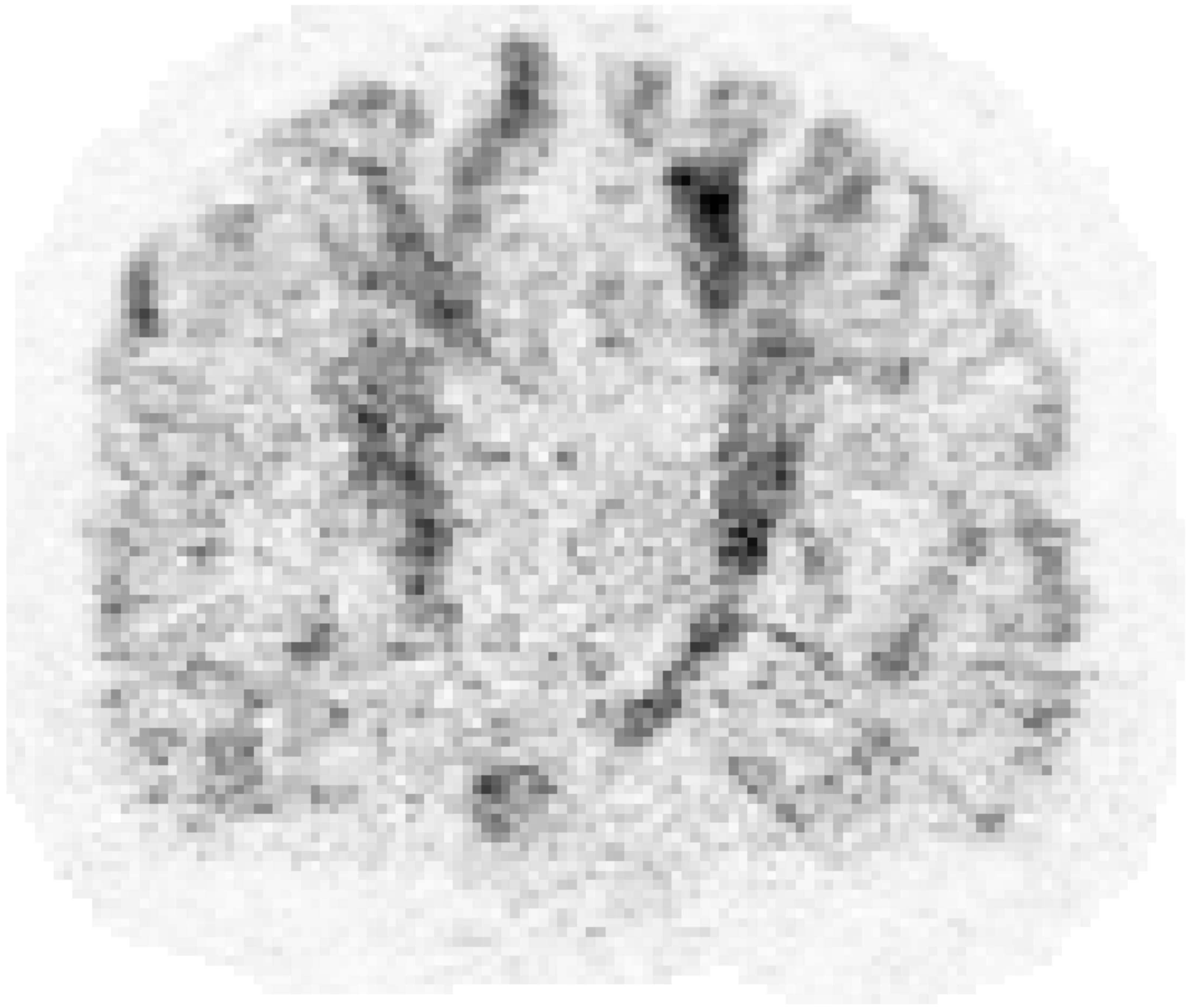


(e) Brain atlas



(f) Diffusion Measurements

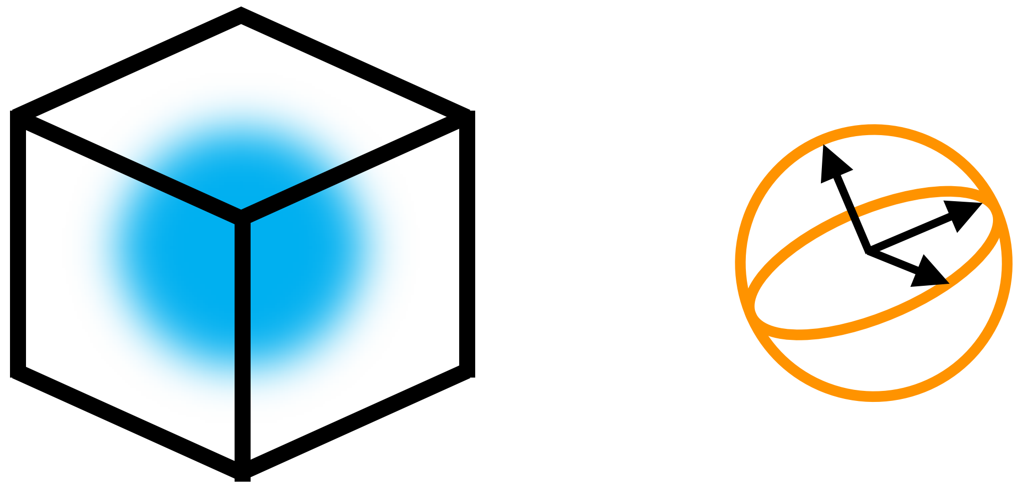
Brain connectivity and Diffusion MRI



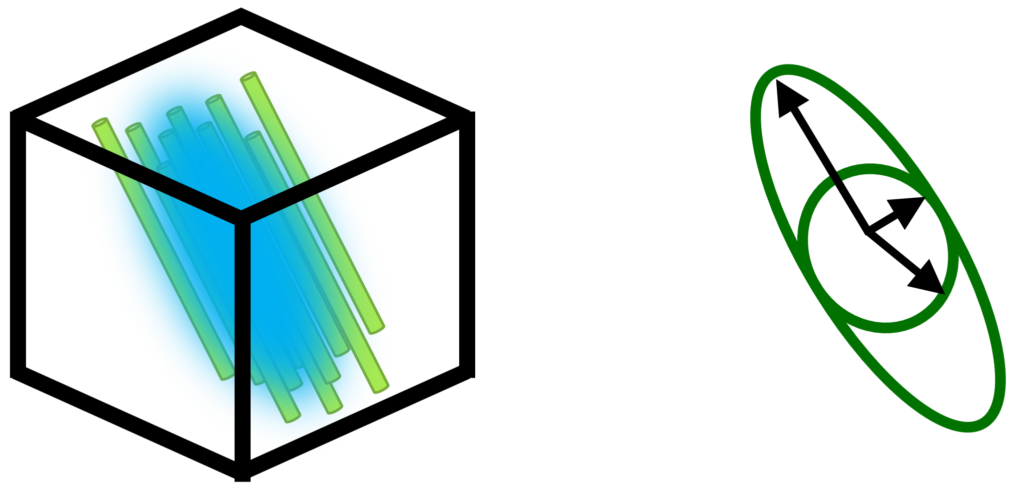
Diffusion MRI

Assessing tissue microstructure using dMRI

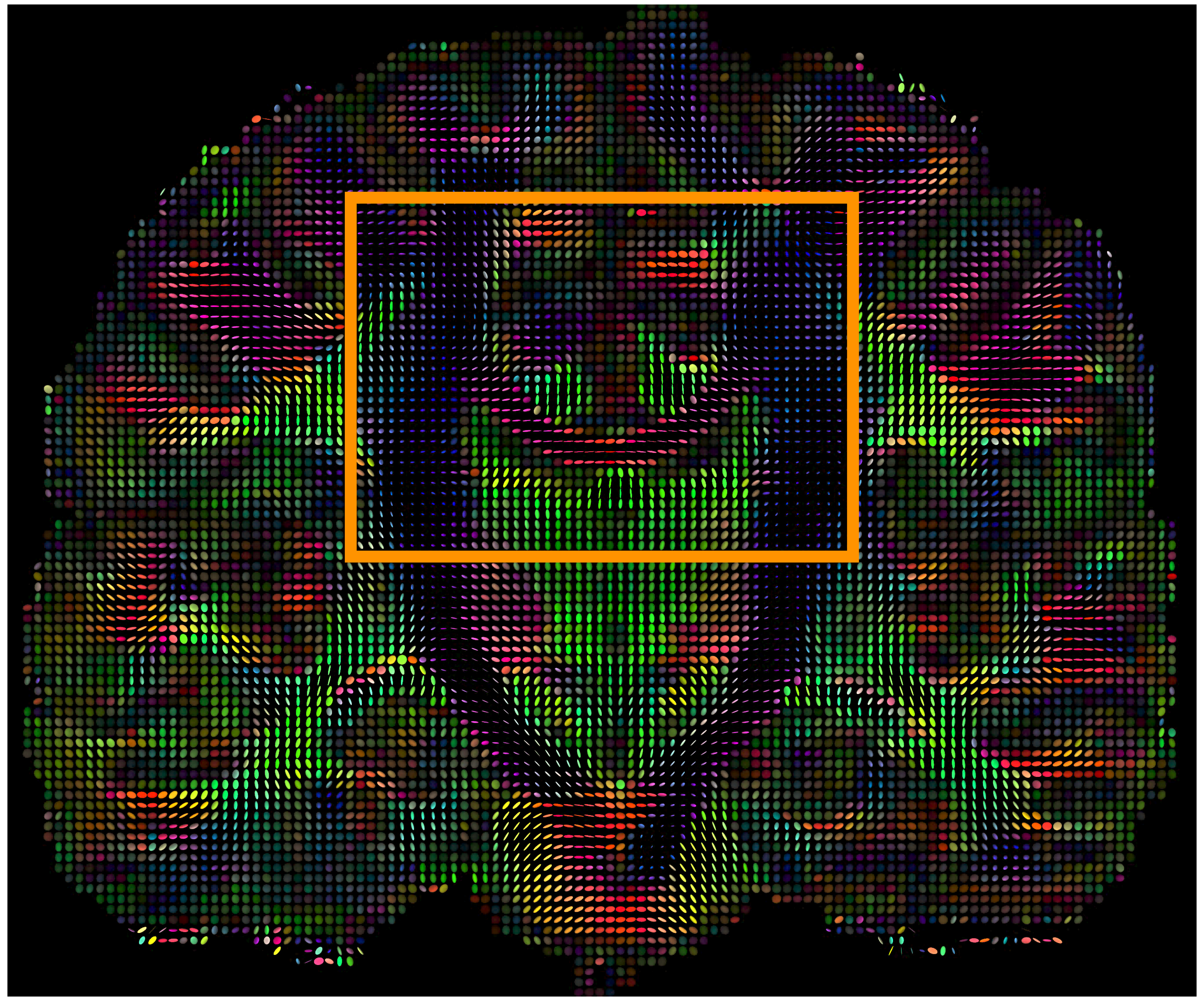
Isotropic diffusion



Anisotropic diffusion

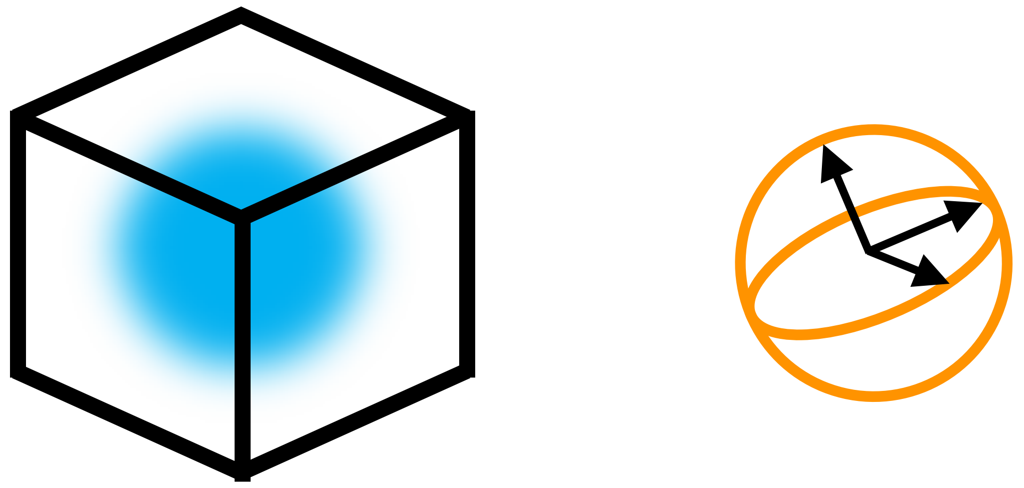


Diffusion tensor imaging (DTI)

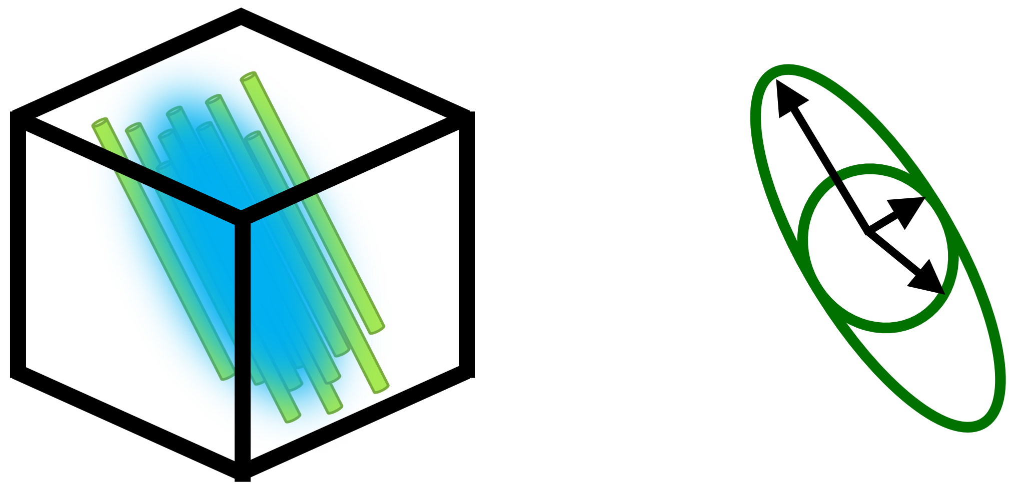


Assessing tissue microstructure using dMRI

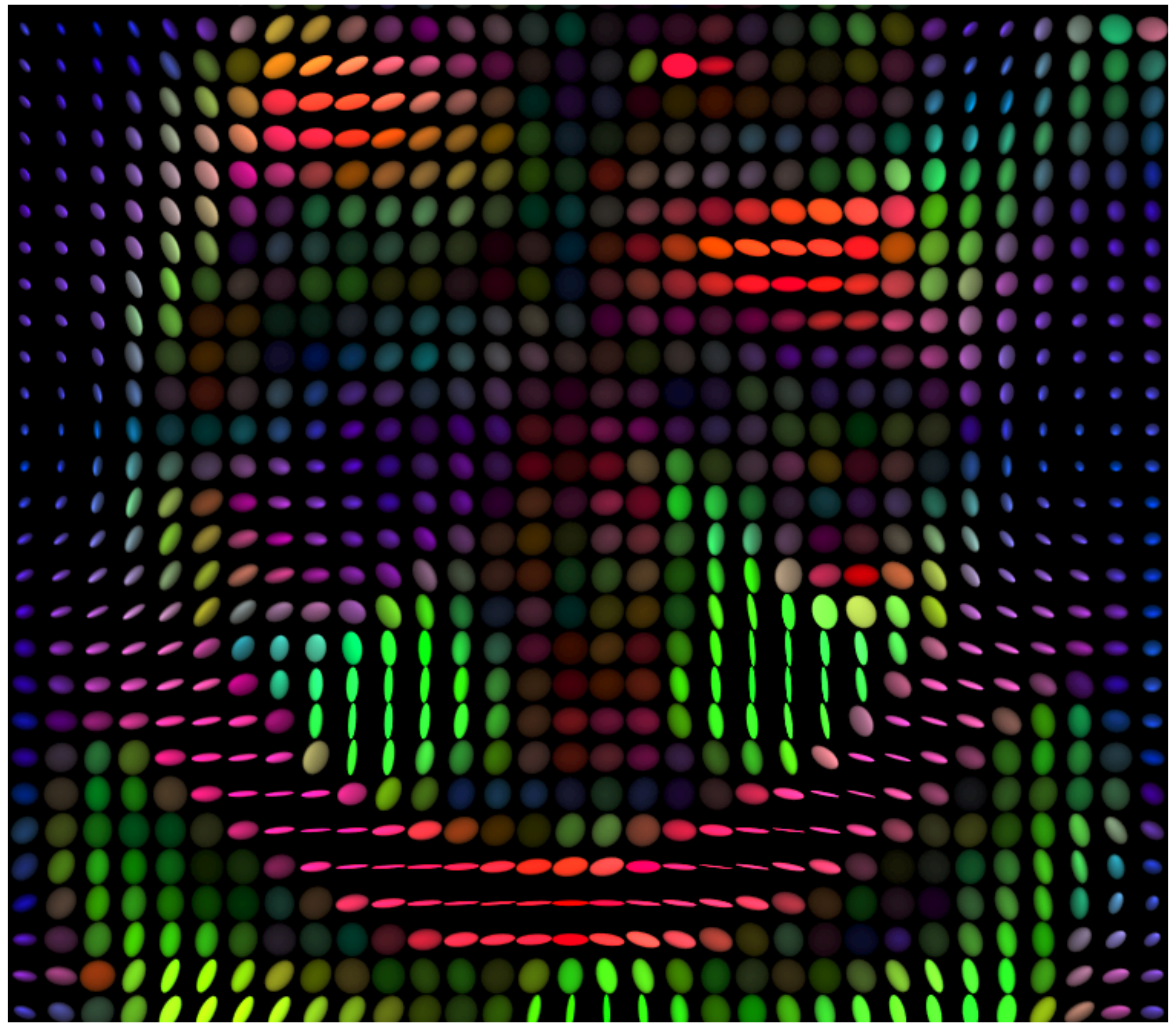
Isotropic diffusion



Anisotropic diffusion

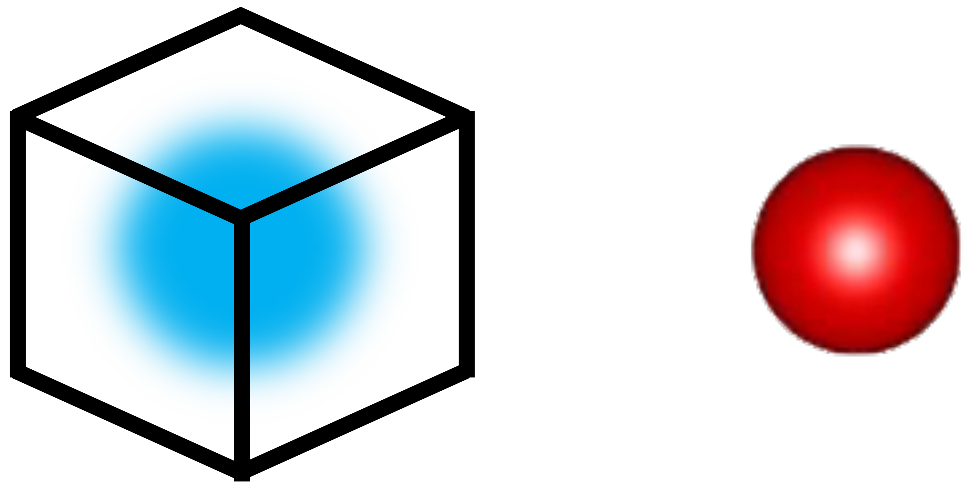


Diffusion tensor imaging (DTI)

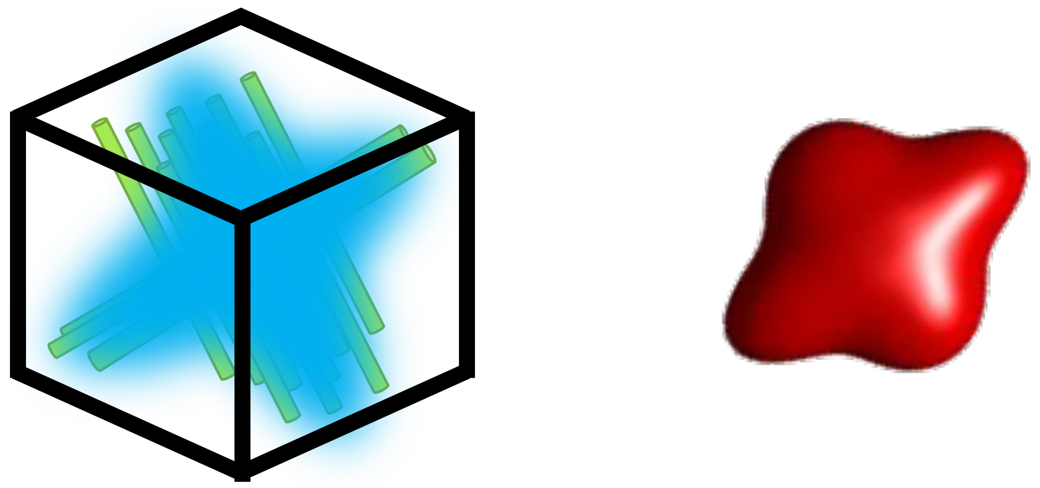


Assessing tissue microstructure using dMRI

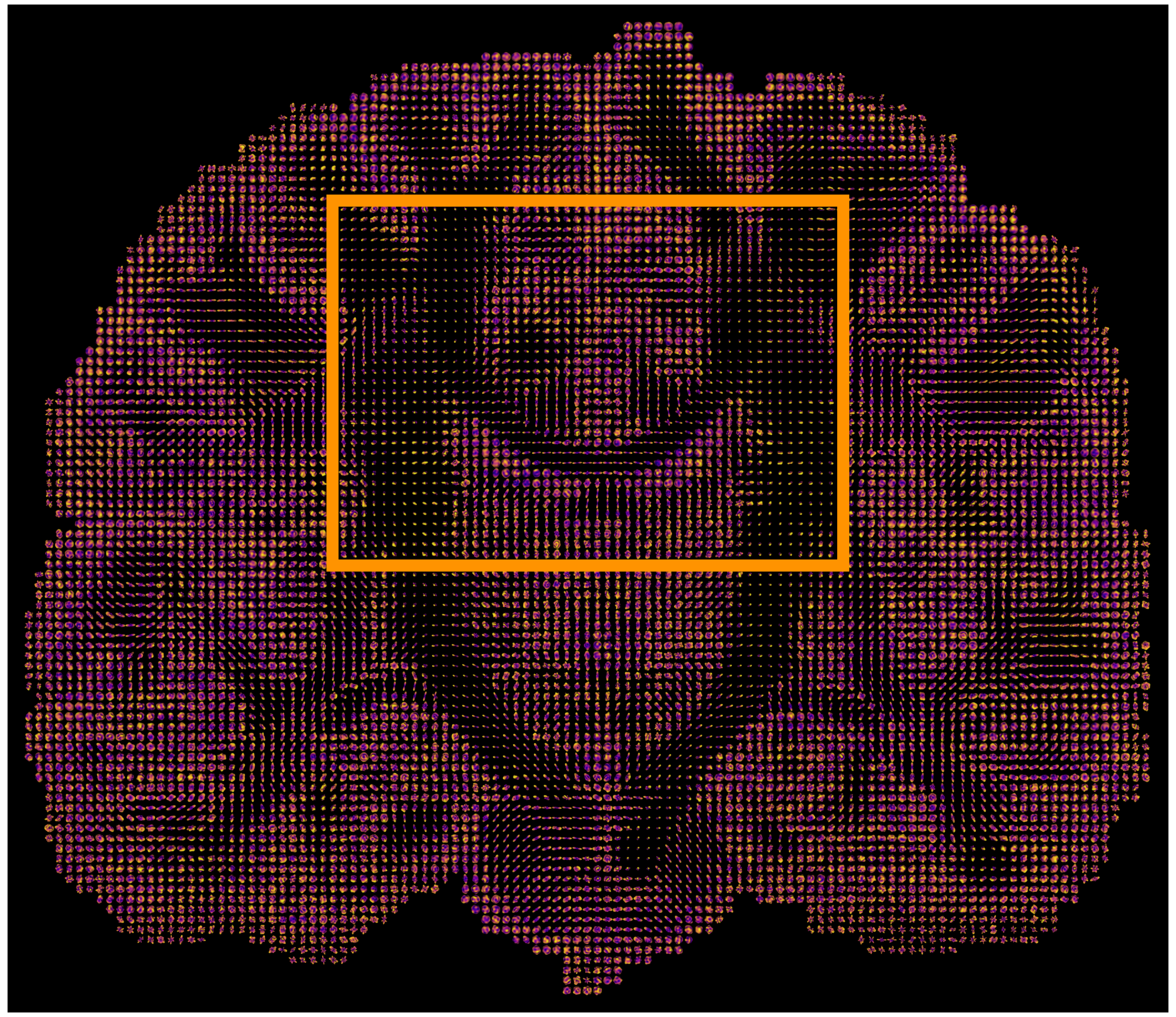
Isotropic diffusion



Anisotropic diffusion

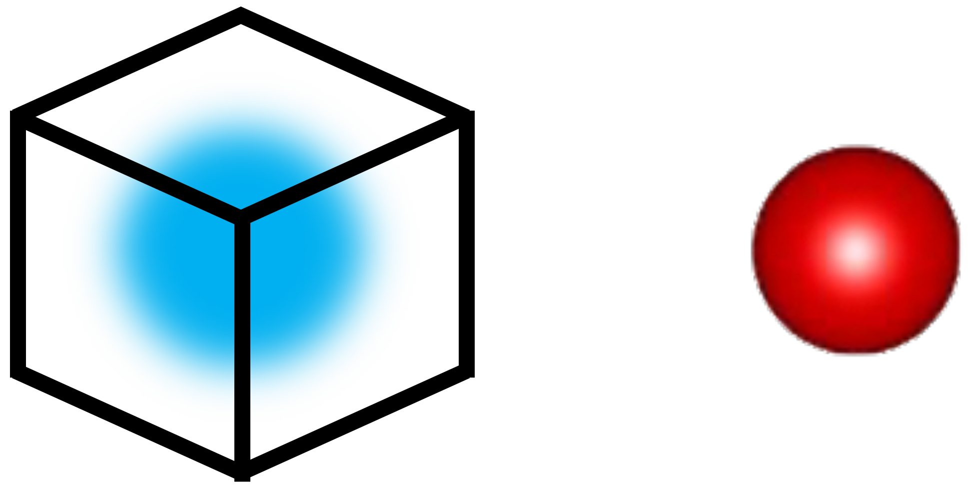


Orientation distribution function (ODF)

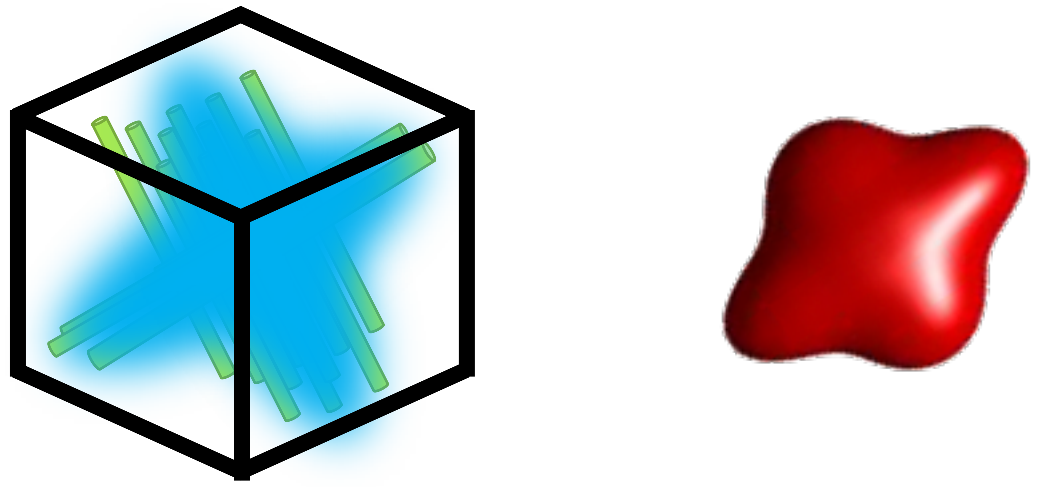


Assessing tissue microstructure using dMRI

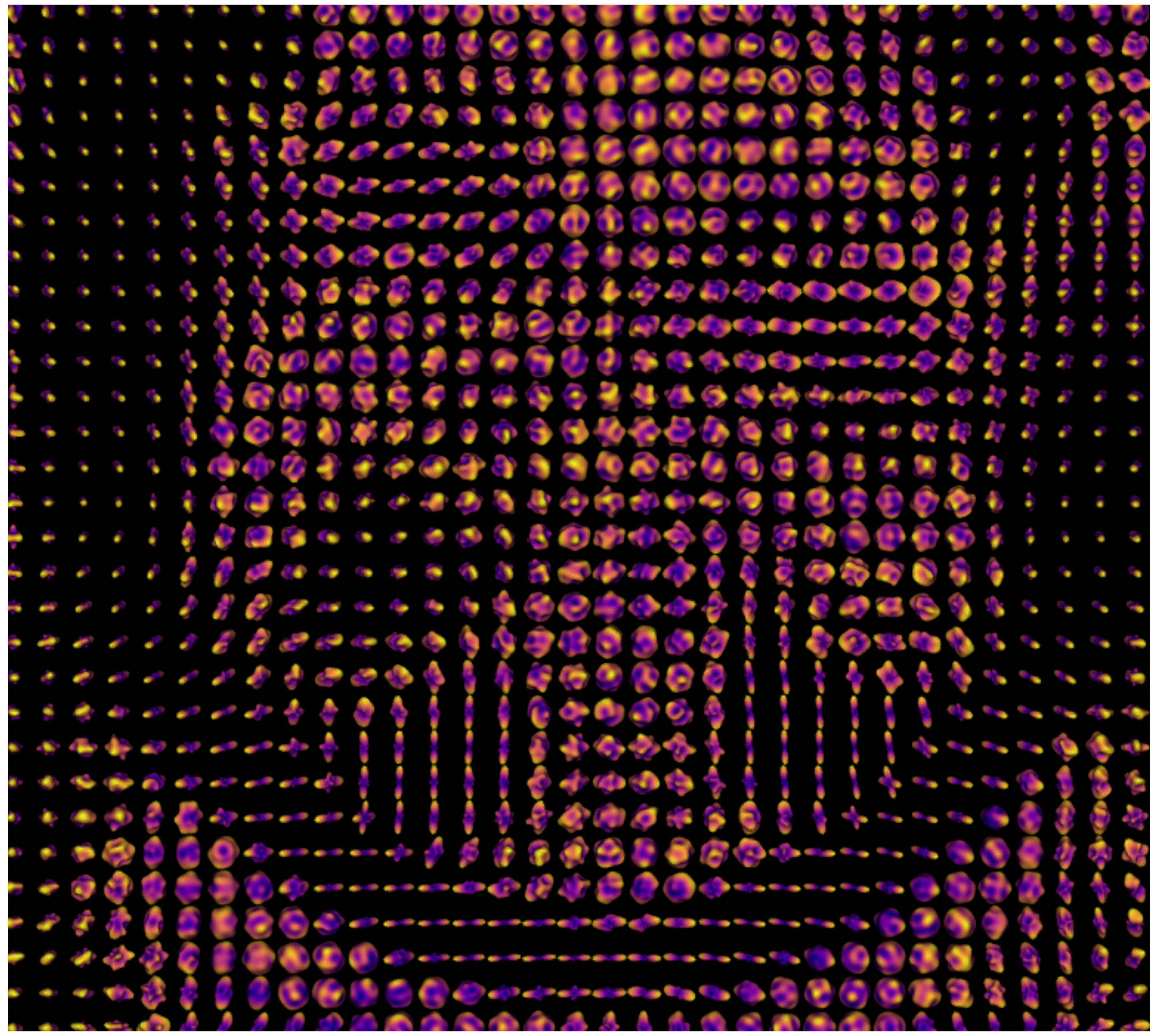
Isotropic diffusion



Anisotropic diffusion

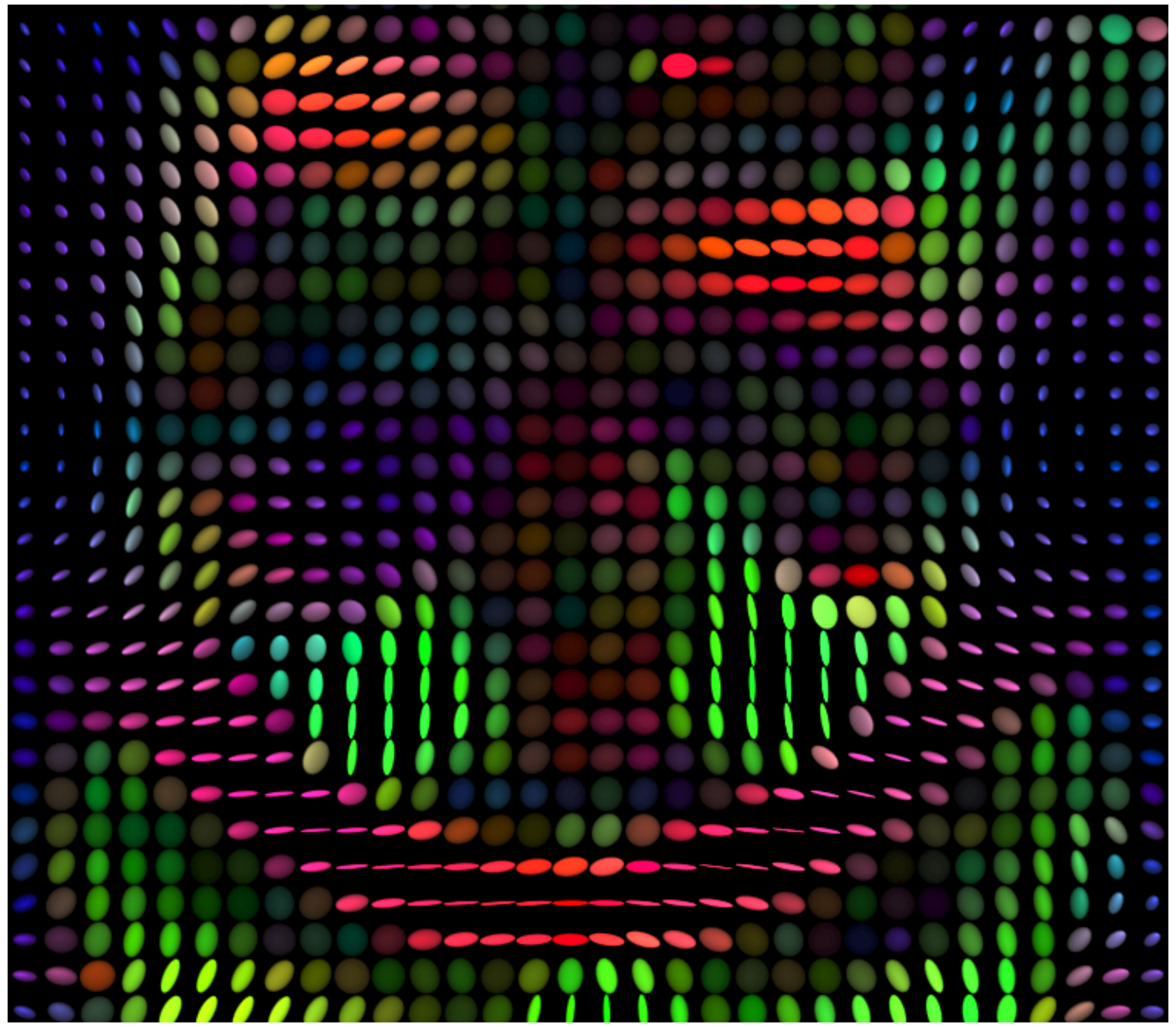


Orientation distribution function (ODF)



Assessing tissue microstructure using dMRI

Diffusion tensor imaging (DTI)



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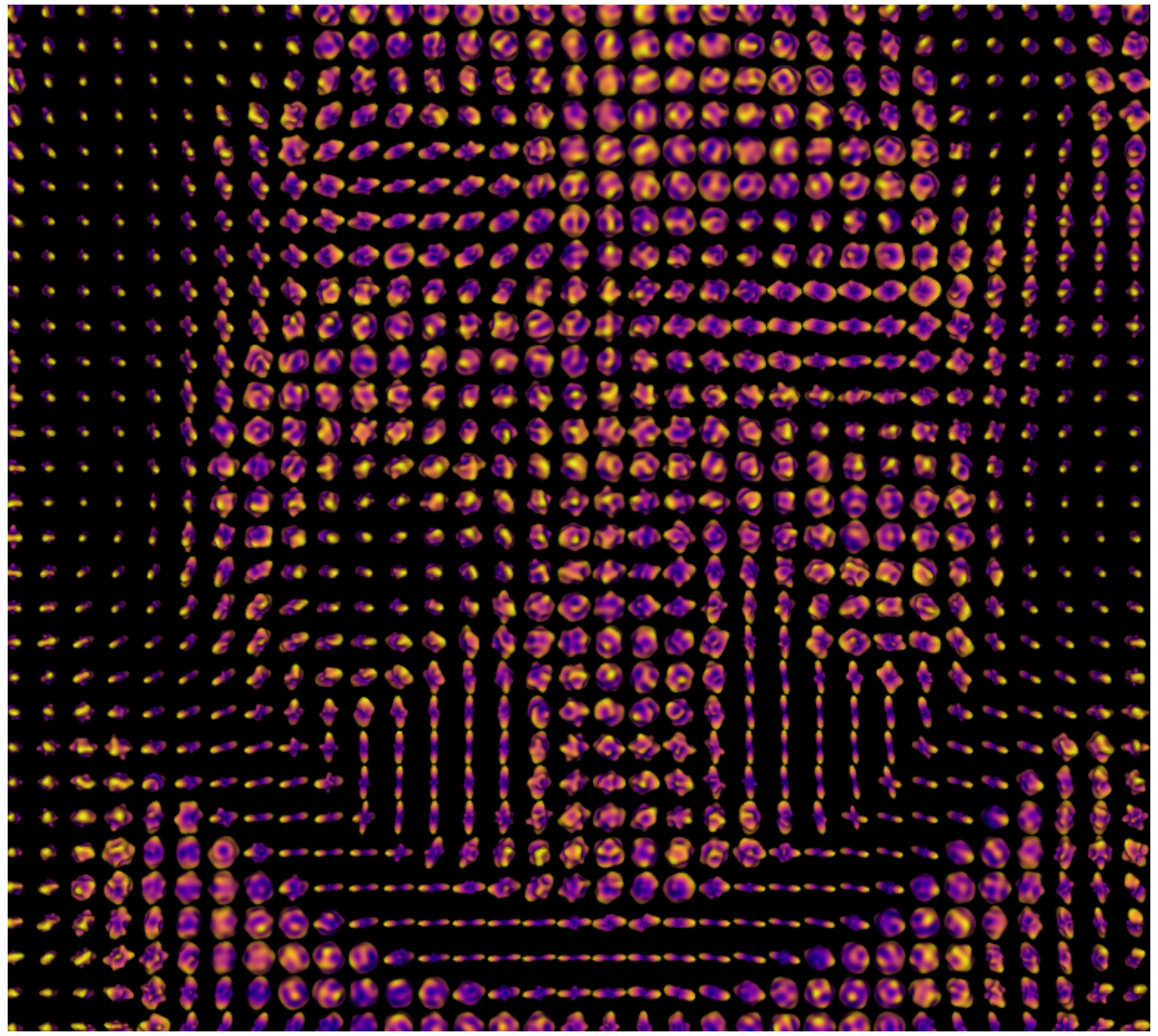
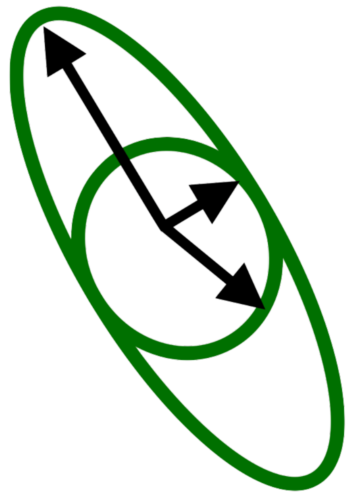


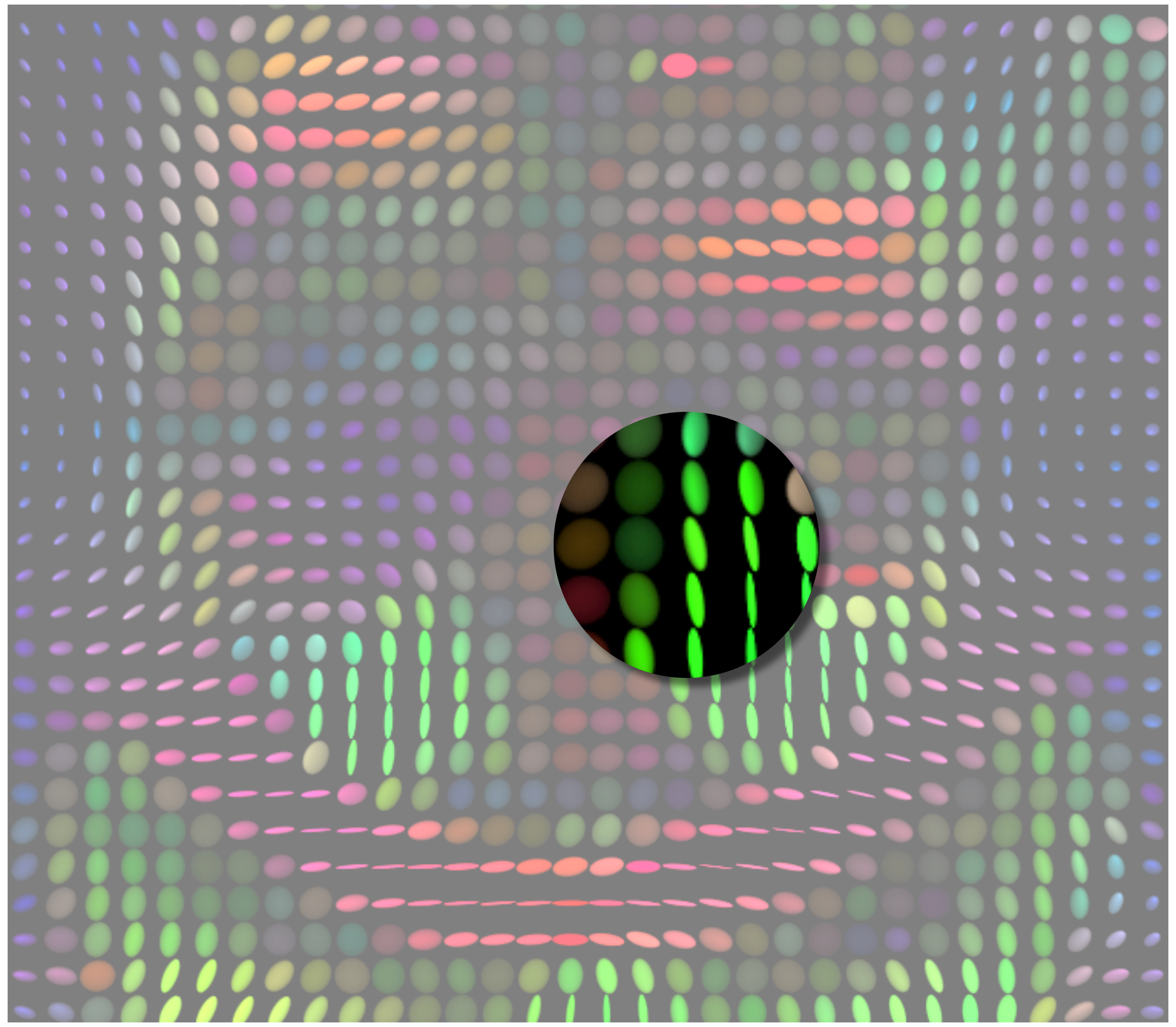
Assessing tissue microstructure using dMRI

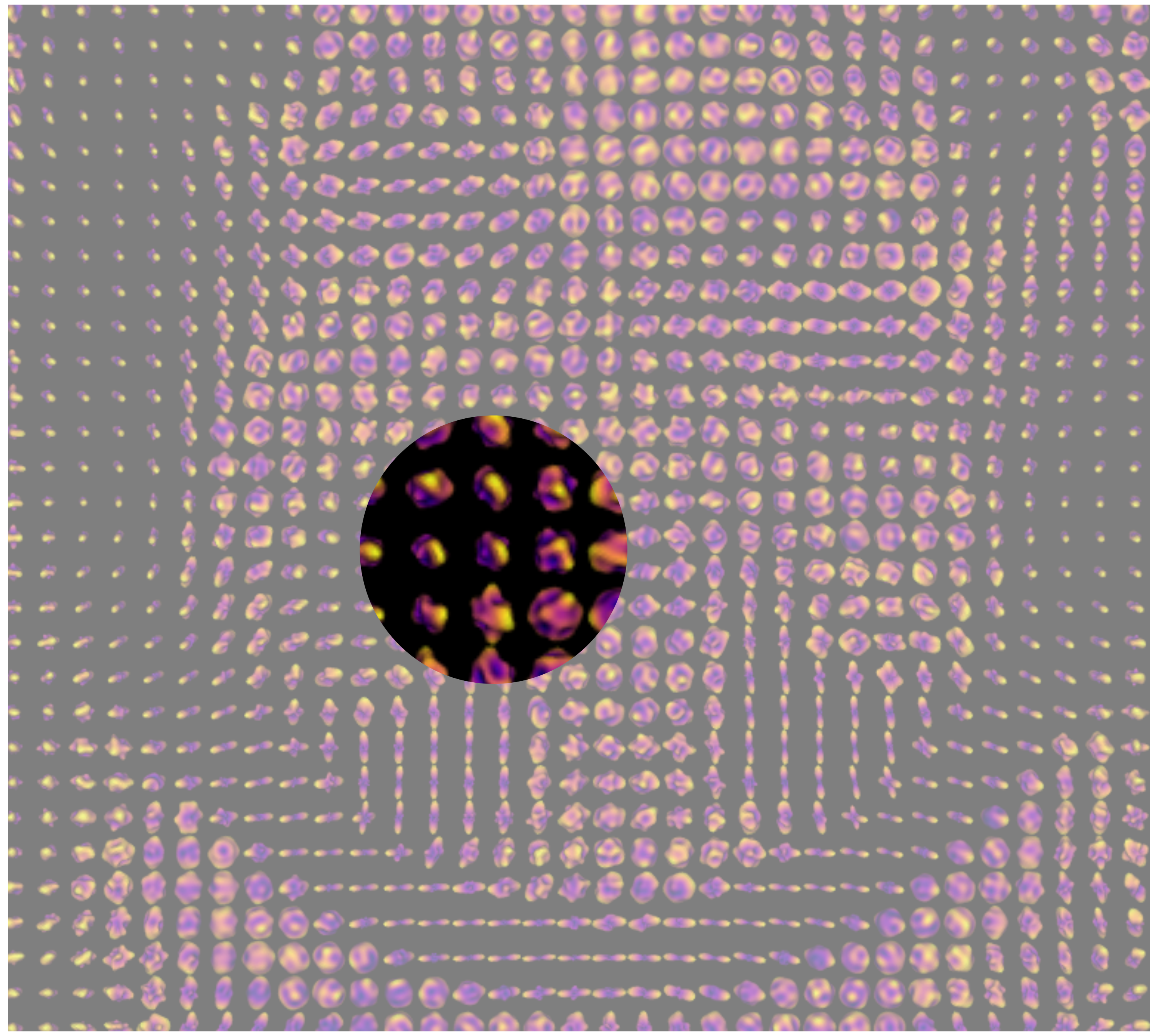
Diffusion tensor imaging (DTI)

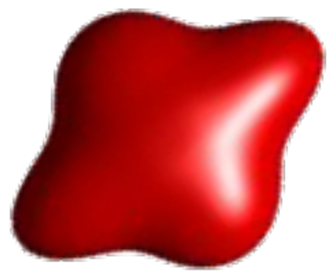
Orientation distribution function (ODF)



SPD(3)







S^{n-1}

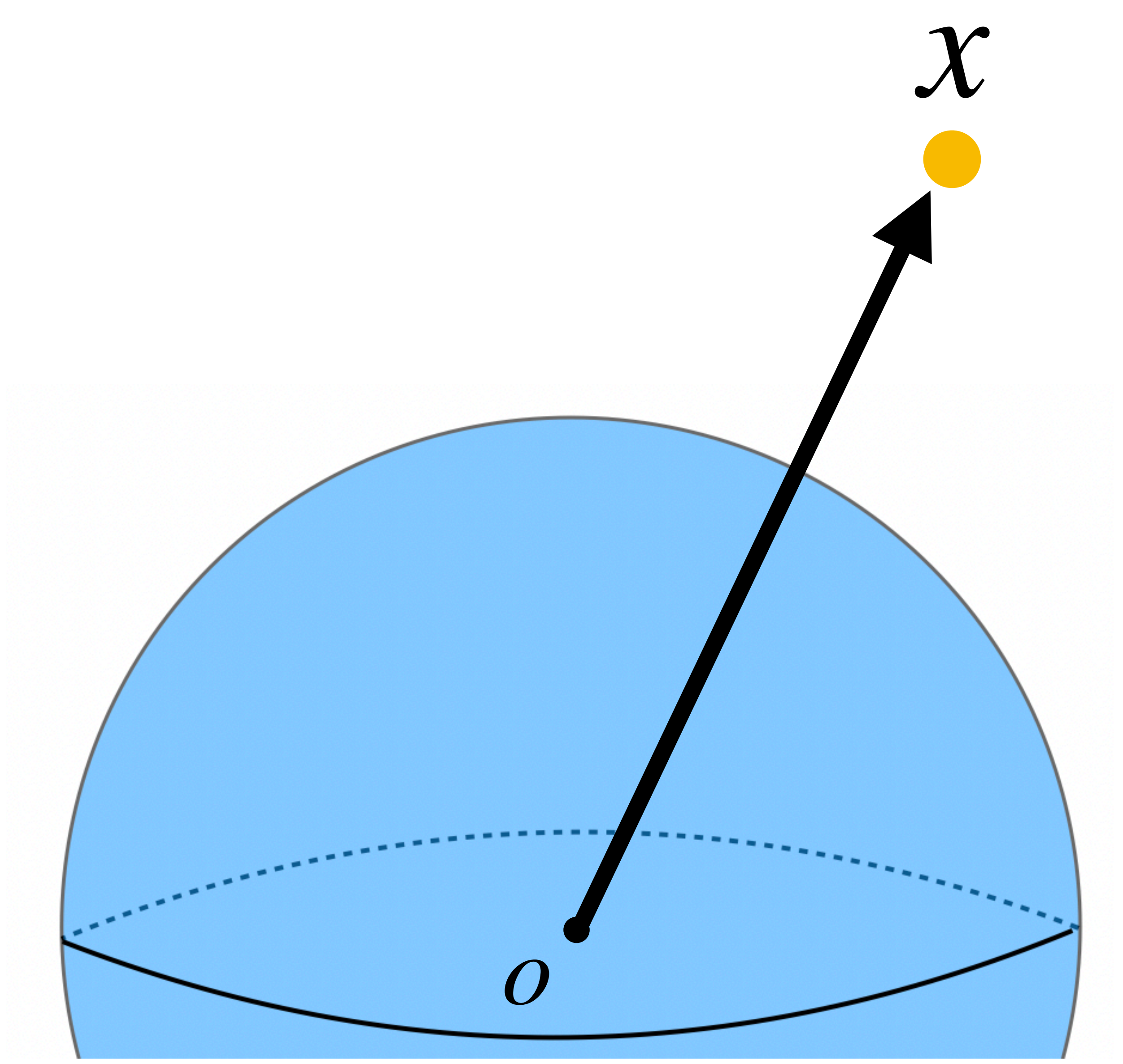
First attempt - Vectorize

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

$$\in SPD$$

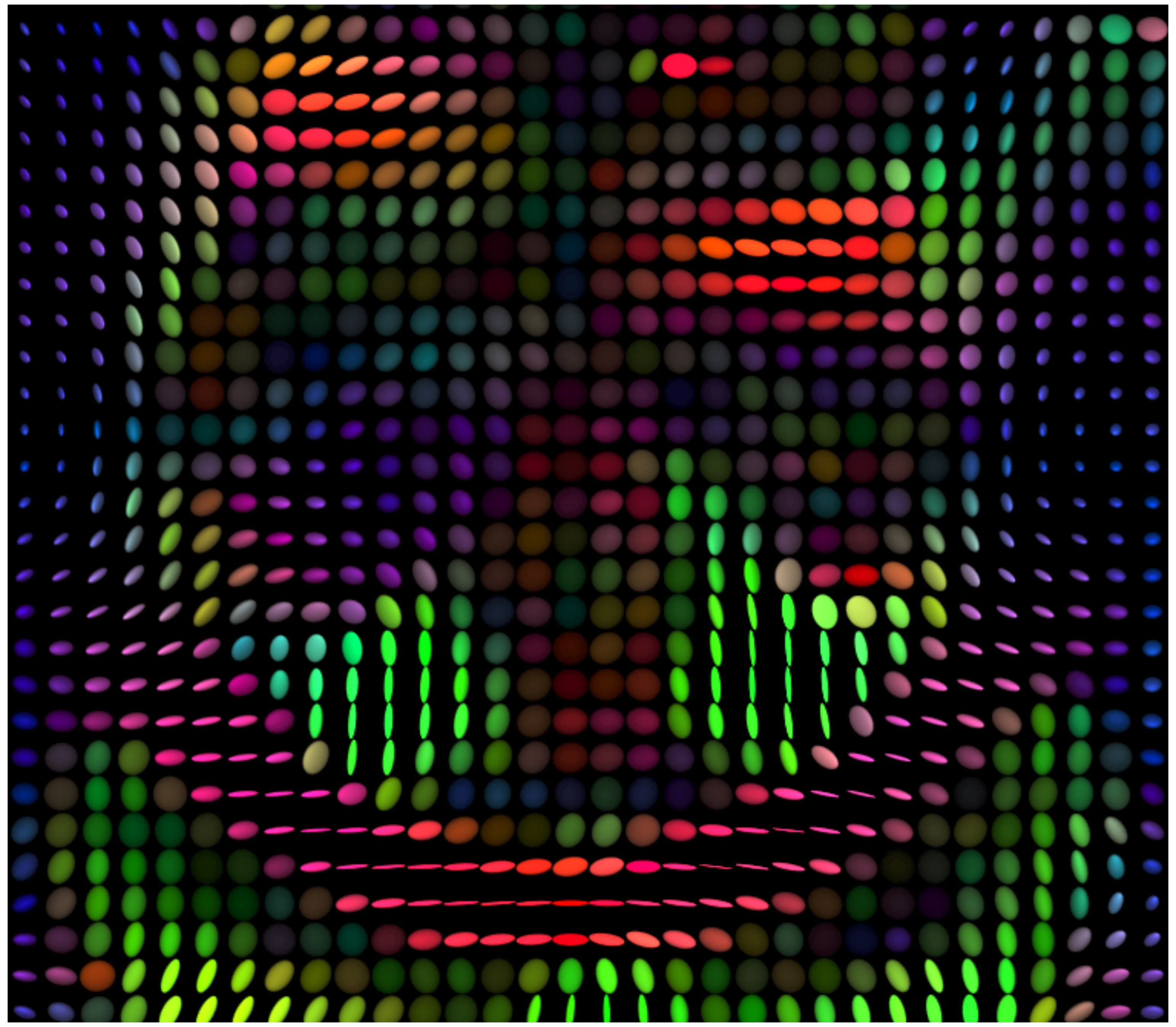
First attempt - Vectorize

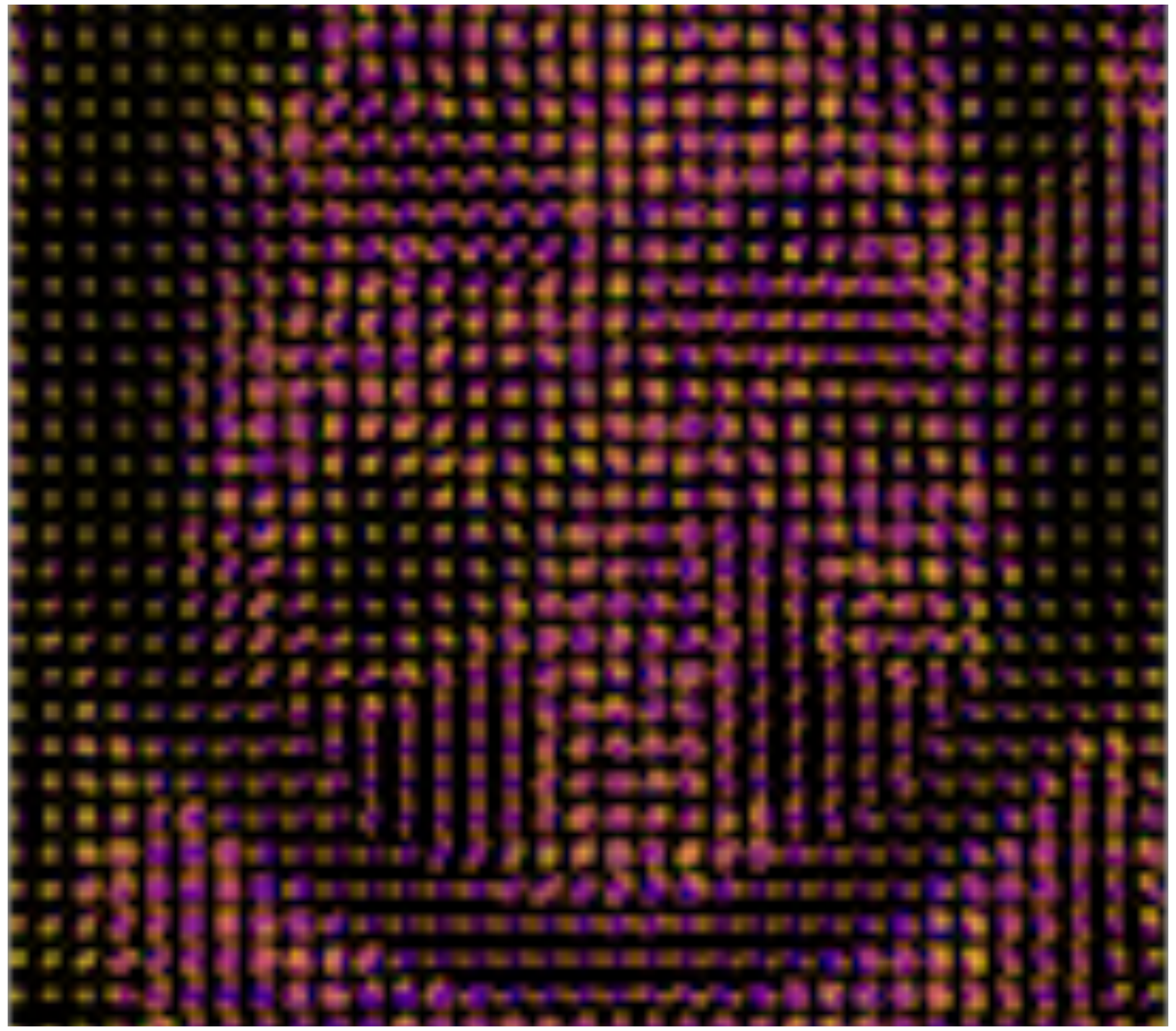
0.2
-0.1
0.02
0.1
0.9
-0.2
0.2
0.3
-0.9
-0.5
-0.8
0.1
0.2
0.1



$\notin S^{n-1}$

First attempt - Convolution



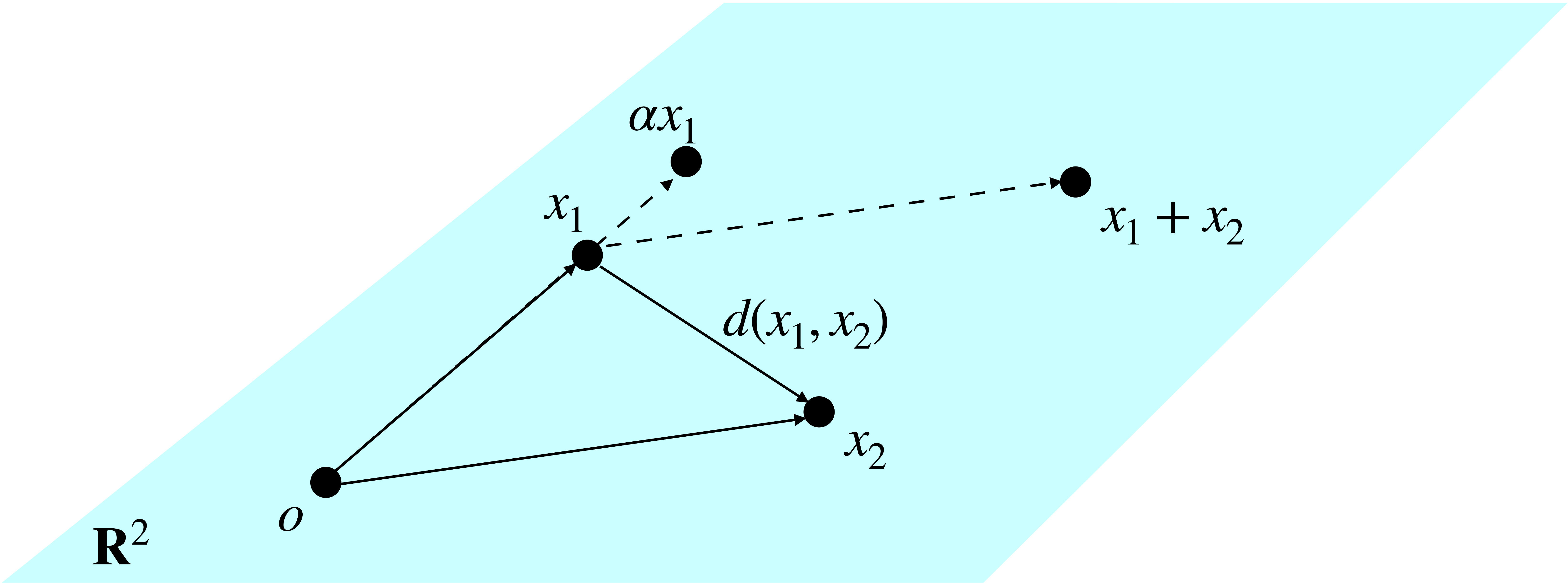


What we need - DTI to ODF

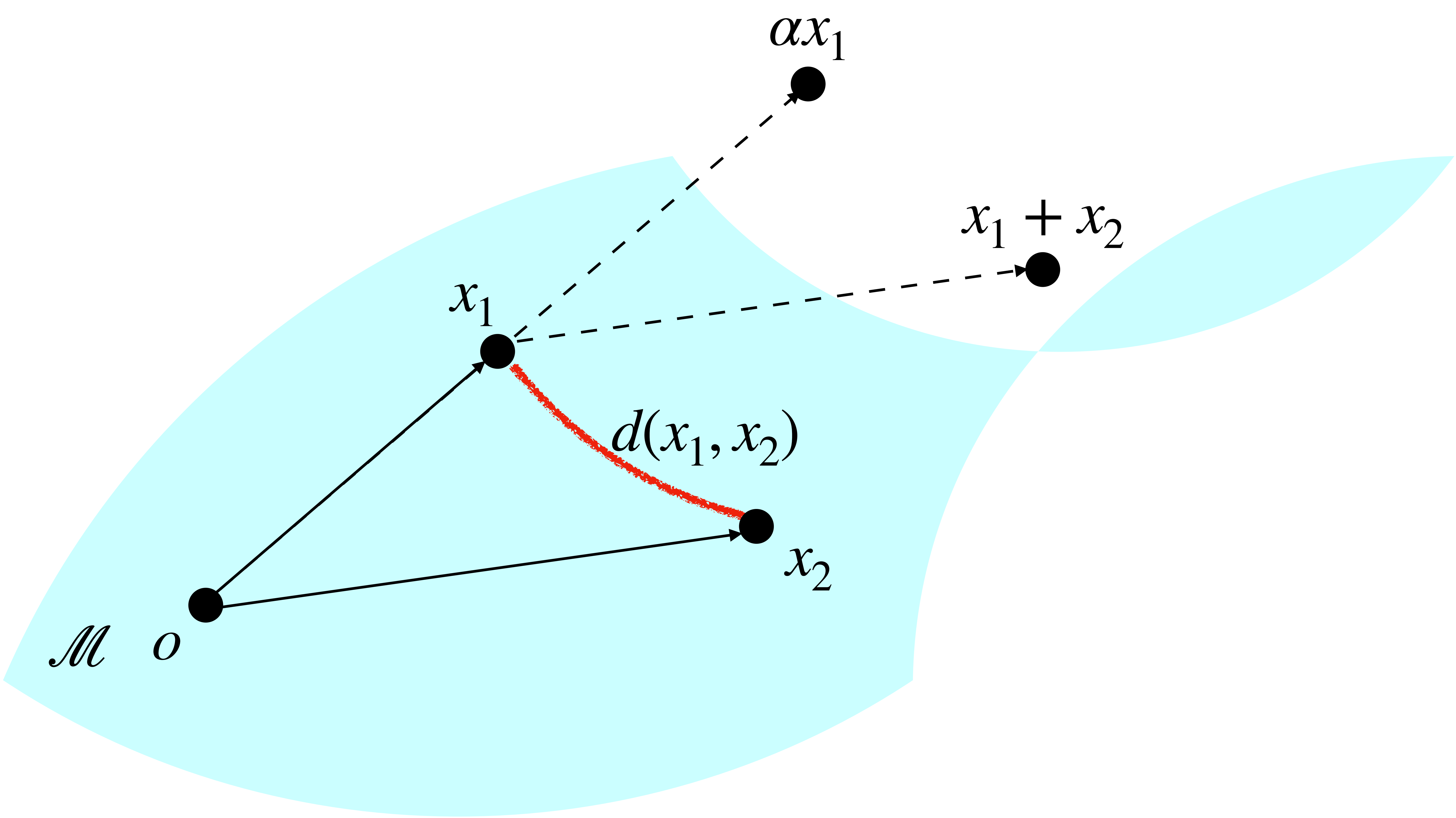
Operators on manifold such that it preserves manifold constraint

A method that can **transfer** modalities between manifolds

Difference between Euclidean and Manifold



Difference between Euclidean and Manifold



From Euclidean to Manifold

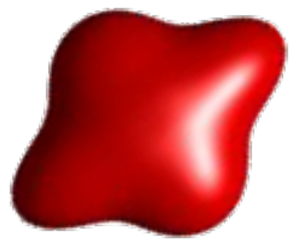
What is **preserved** in Manifold from Euclidean space?

How to make minimum **modifications** on unpreserved parts from Euclidean space to Manifold?

The operators needed for Manifold

Main calculation in deep learning

$$y = \sigma(Wx + b)$$

Where x, y are 

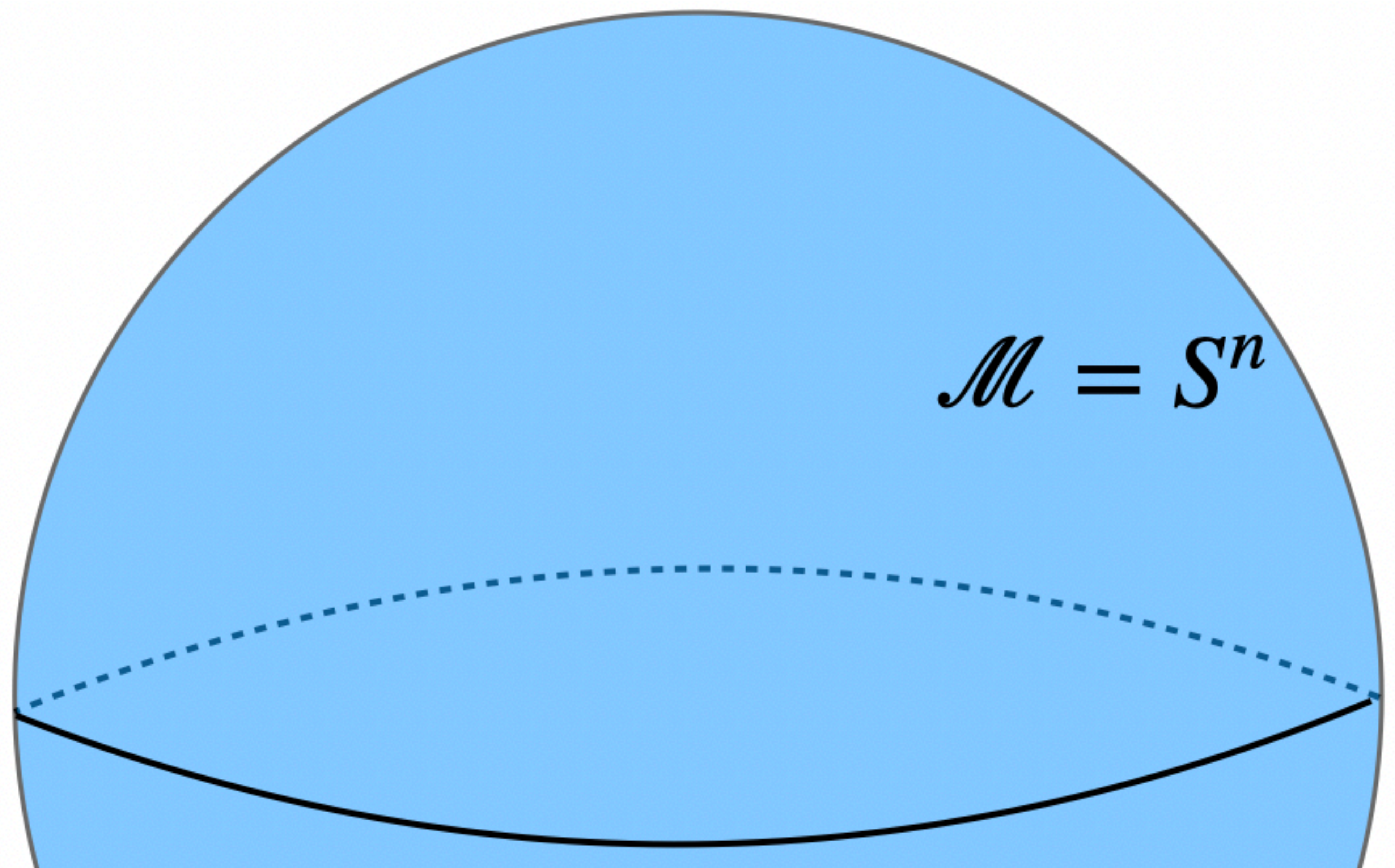
Multiplication $\times$

Addition $+$

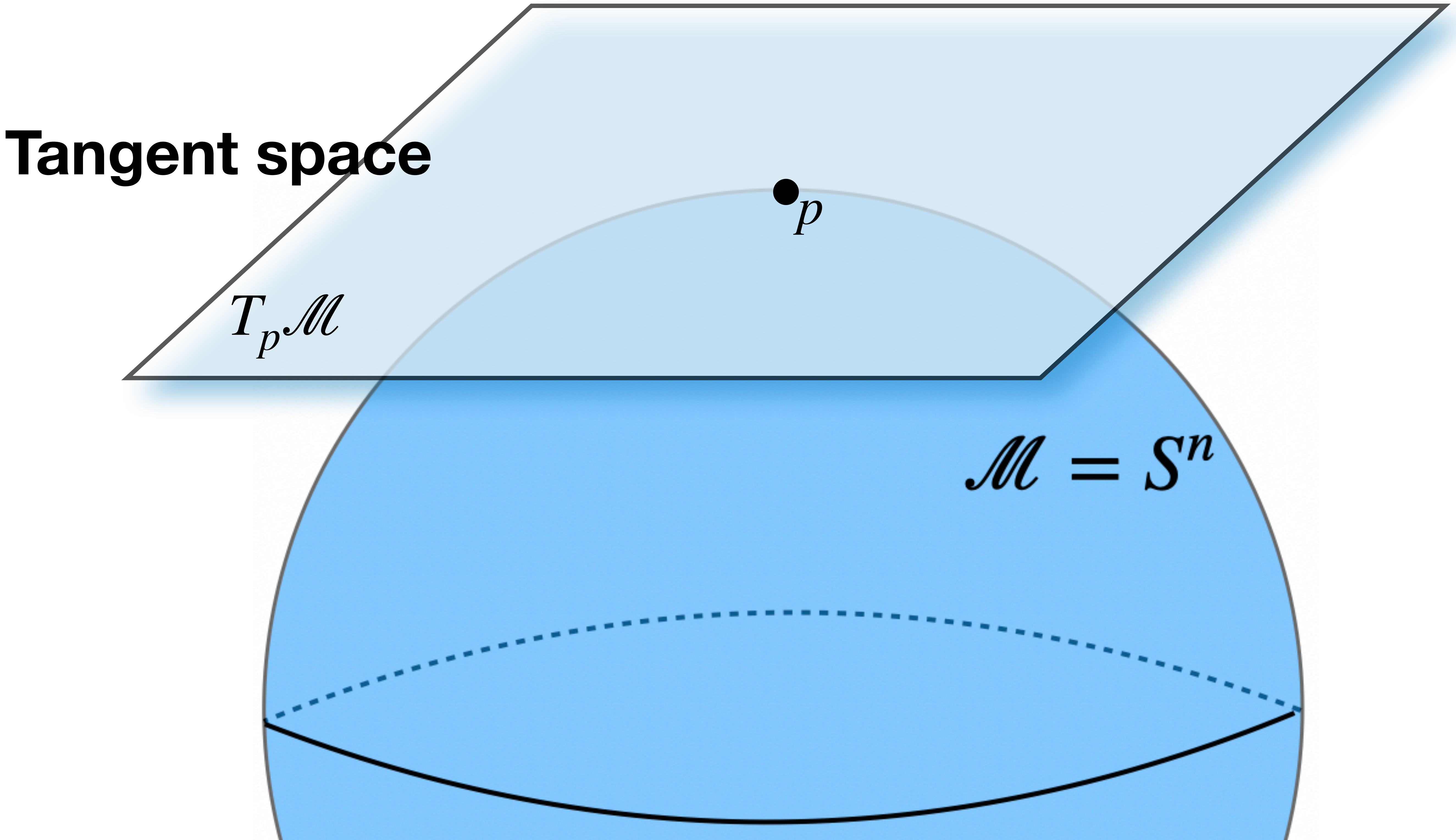
Activation

The operators needed for Manifold

The operators needed for Manifold



The operators needed for Manifold



The operators needed for Manifold

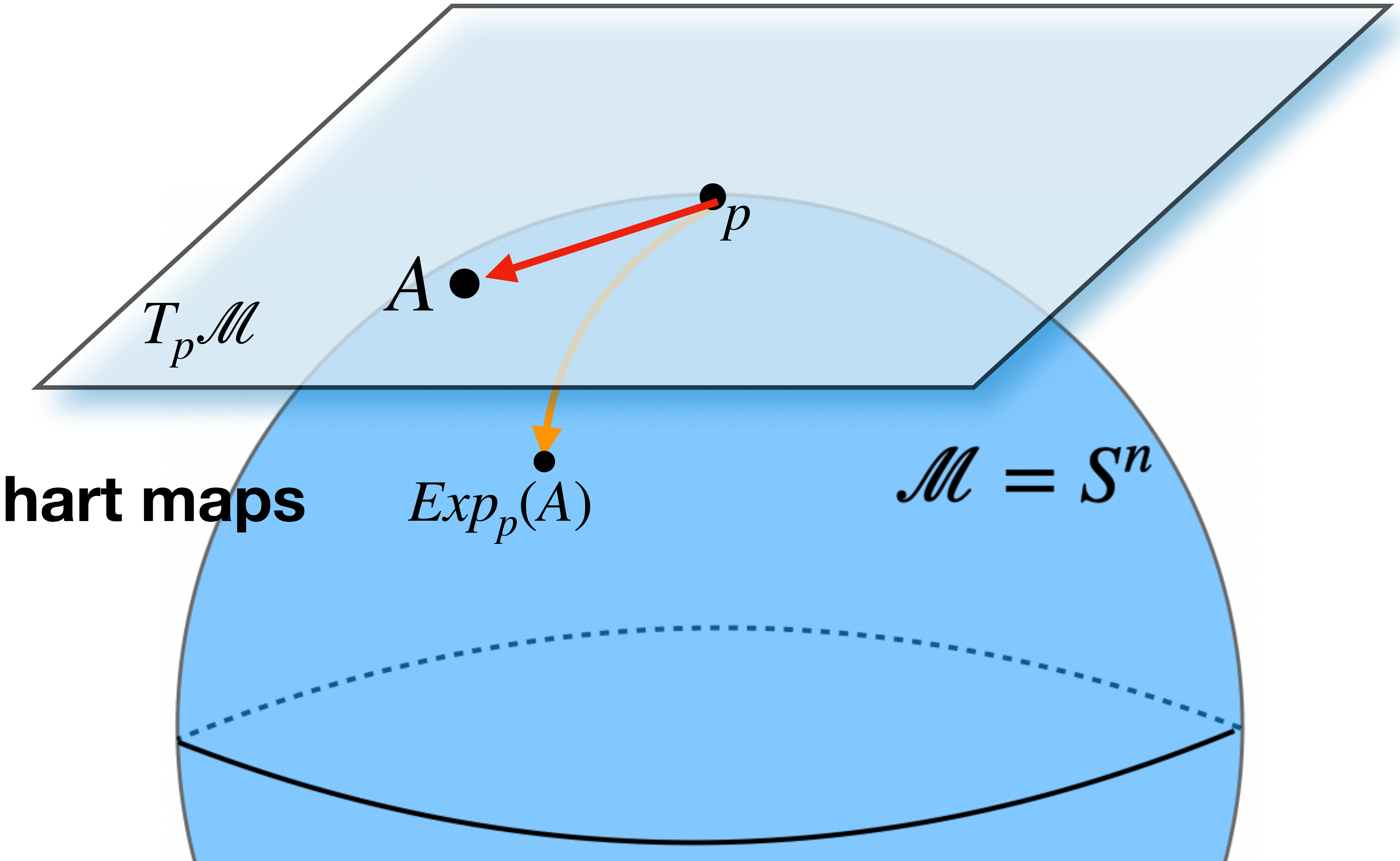
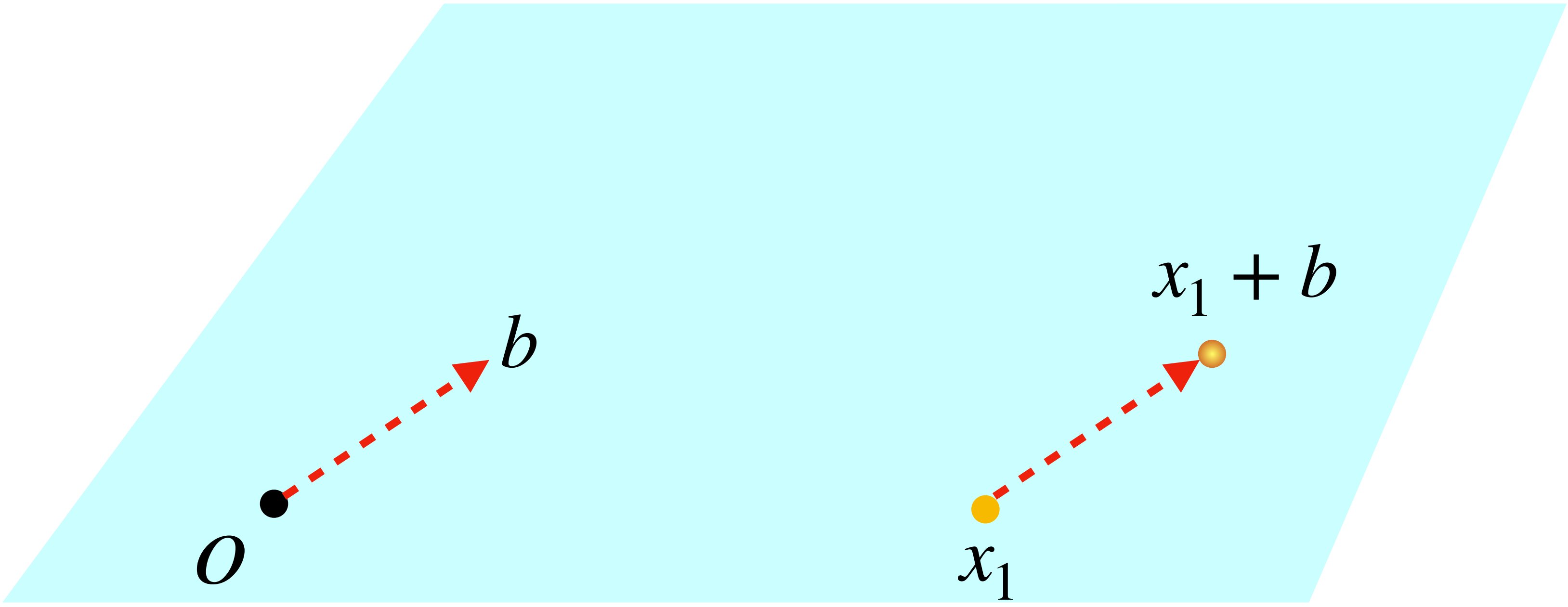
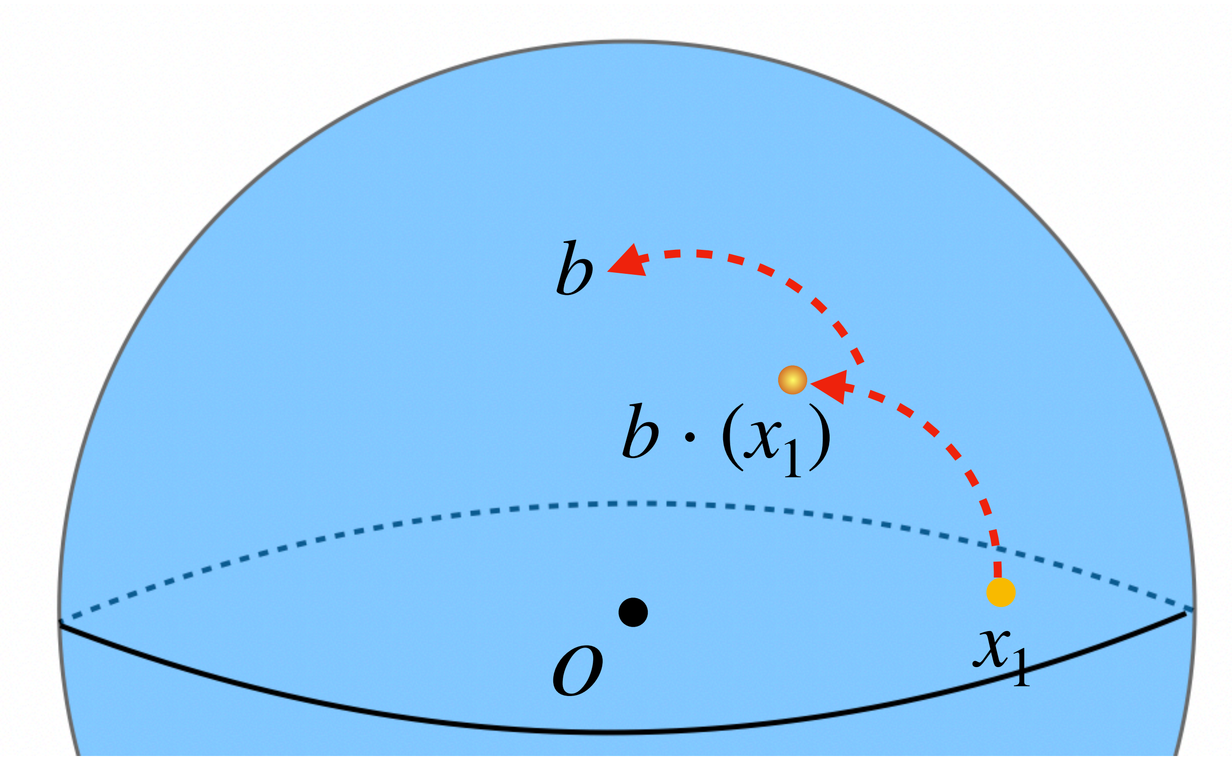


Chart maps

The operators needed for Manifold

Group operations: A diffeomorphism ϕ, if $d(\phi(x), \phi(y)) = d(x, y)$





What we need - DTI to ODF

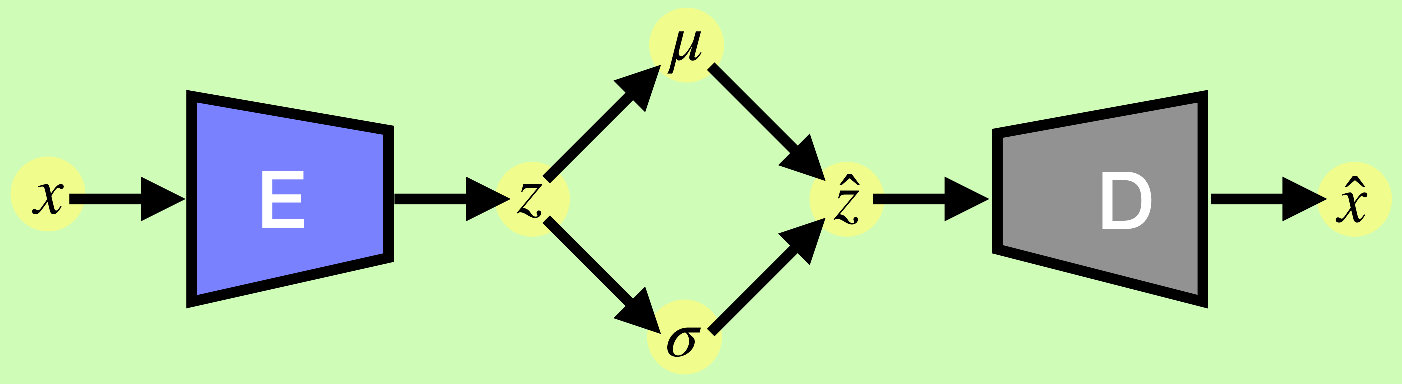
Operators on manifold such that it preserves manifold constraint

A method that can **transfer** modalities between manifolds

Generative model

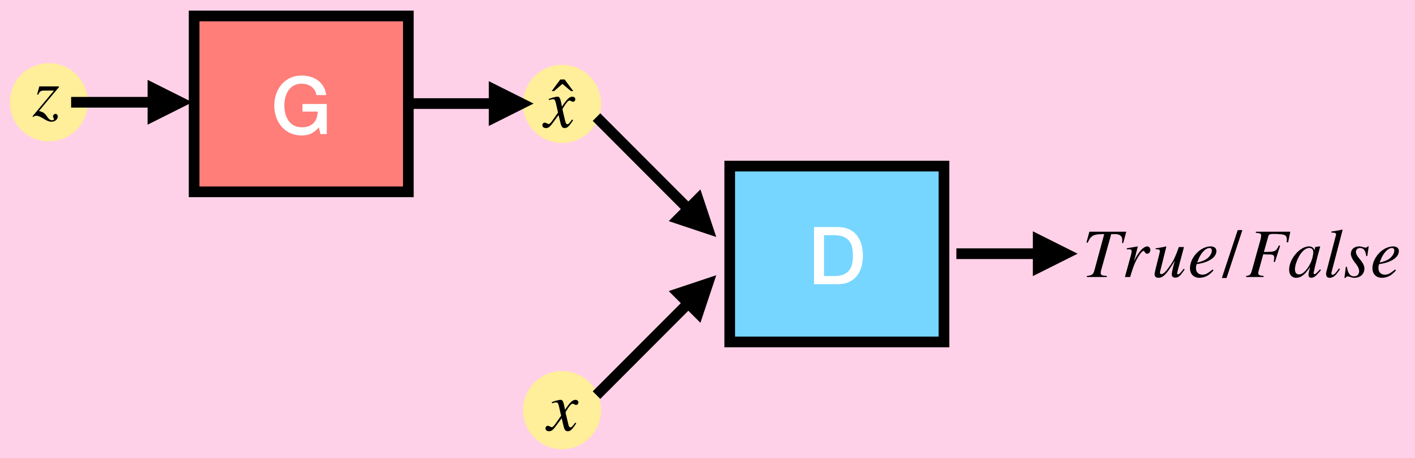
Variational autoencoder (VAE)

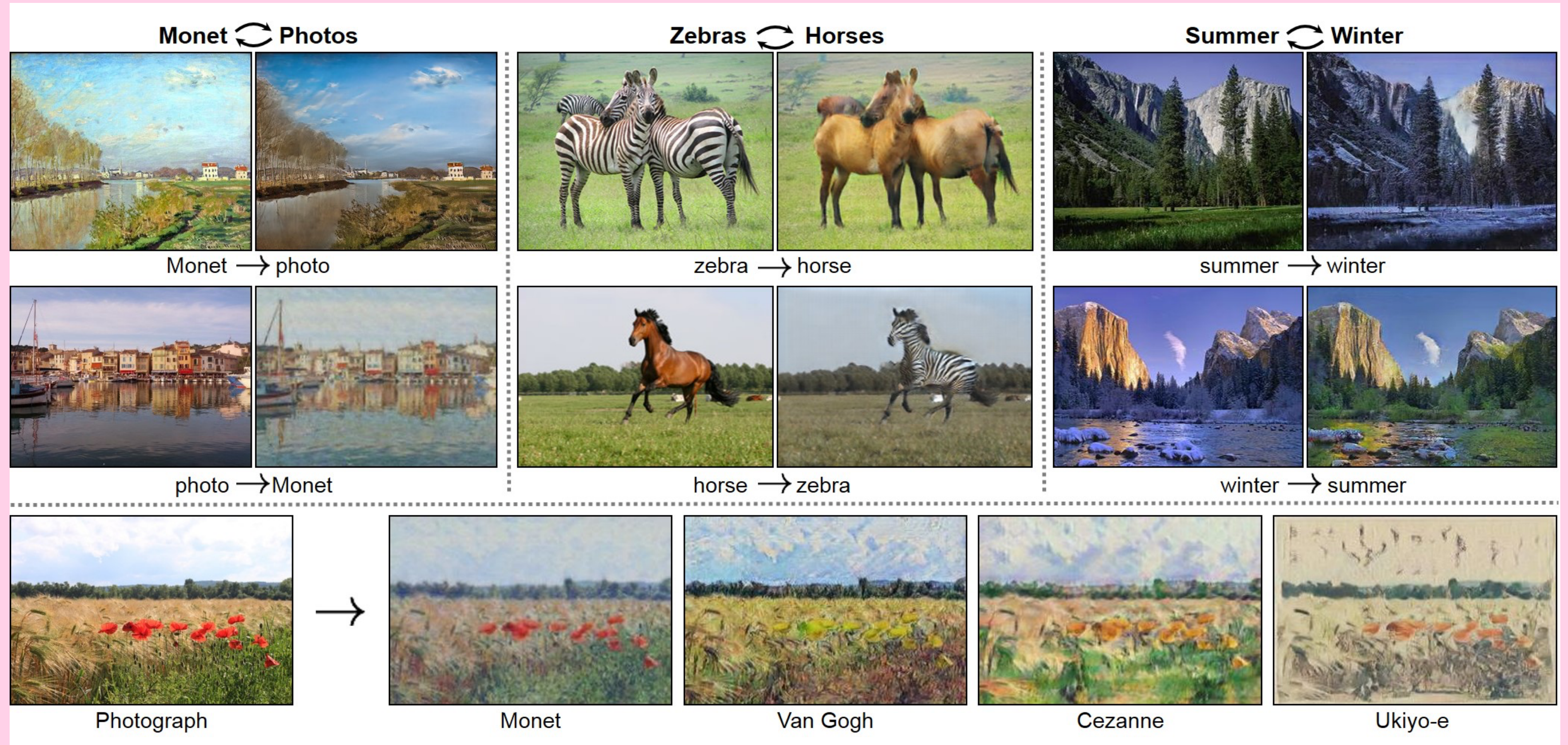
$$l_i(\theta, \phi) = -\mathbf{E}_{z\sim q_\theta(z|x_i)}[logp_\phi(x_i|z)] + \mathbf{KL}(q_\theta(z|x_i)||p(z))$$



Generative adversarial network (GAN)

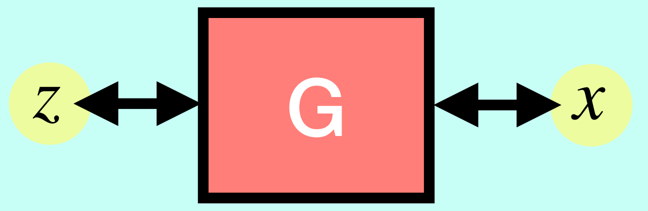
$$\min_G \max_D V(D, G) = \mathbf{E}_{x\sim p_{data}(x)}[logD(x)] + \mathbf{E}_{z\sim p_z(z)}[log(1 - D(G(z)))]$$

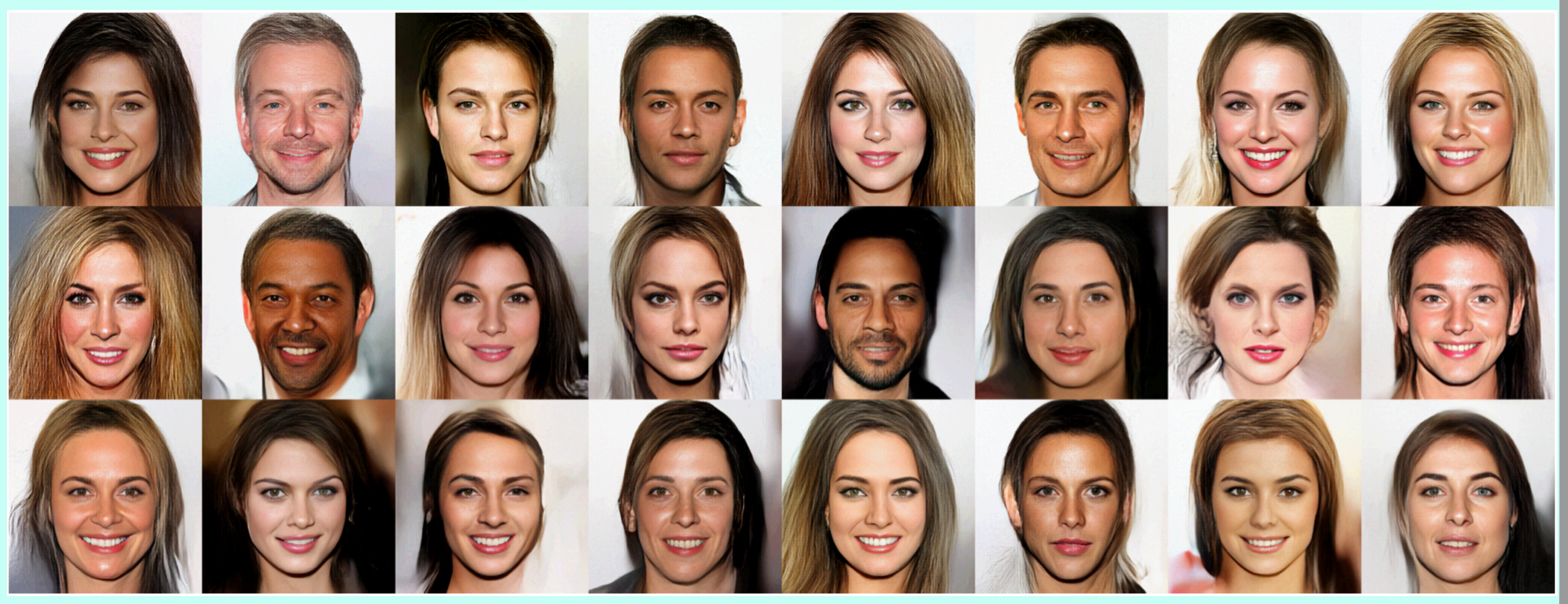




Normalizing flows

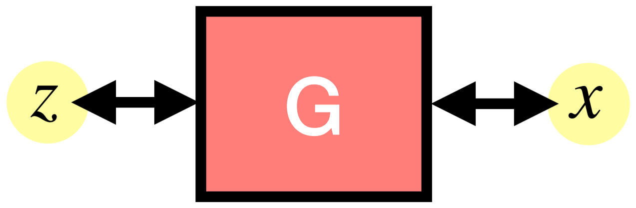
$$\min l(\mathcal{D}) = \frac{1}{N}\sum_{i=1}^{N} - logp_\theta(x^{(i)}), z \sim p_\theta(z), x = g_\theta(z), z = g_\theta^{-1}(x)$$





VQ-VAE-2, Razavi, etc. Cycle GAN, Zhu, etc. GLOW, Kingma, etc.

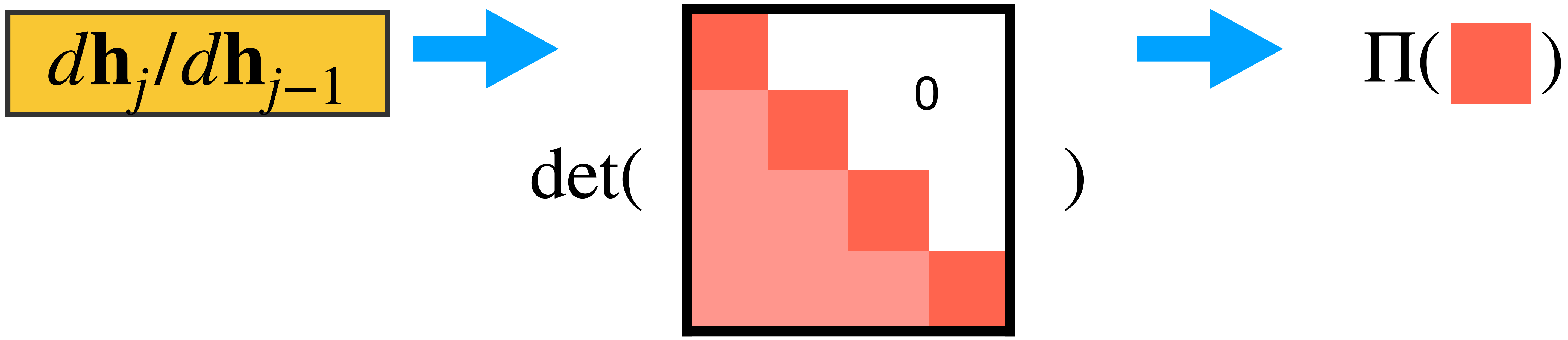
Normalizing Flow



Normalizing Flow

$$z \leftrightarrow L_4 \leftrightarrow h_3 \leftrightarrow L_3 \leftrightarrow h_2 \leftrightarrow L_2 \leftrightarrow h_1 \leftrightarrow L_1 \leftrightarrow x$$

$$\log p_\theta(\mathbf{x}) = \log p(\mathbf{z}) + \log|\det(d\mathbf{z}/d\mathbf{x})| = \log p_\theta(\mathbf{z}) + \sum_{j=0}^{K} \log|\det(d\mathbf{h}_j/d\mathbf{h}_{j-1})|$$



Normalizing Flow - Basic Structures

Actnorm

$$Y = \frac{1}{\sigma} \odot (X - \mu)$$

1×1 convolution

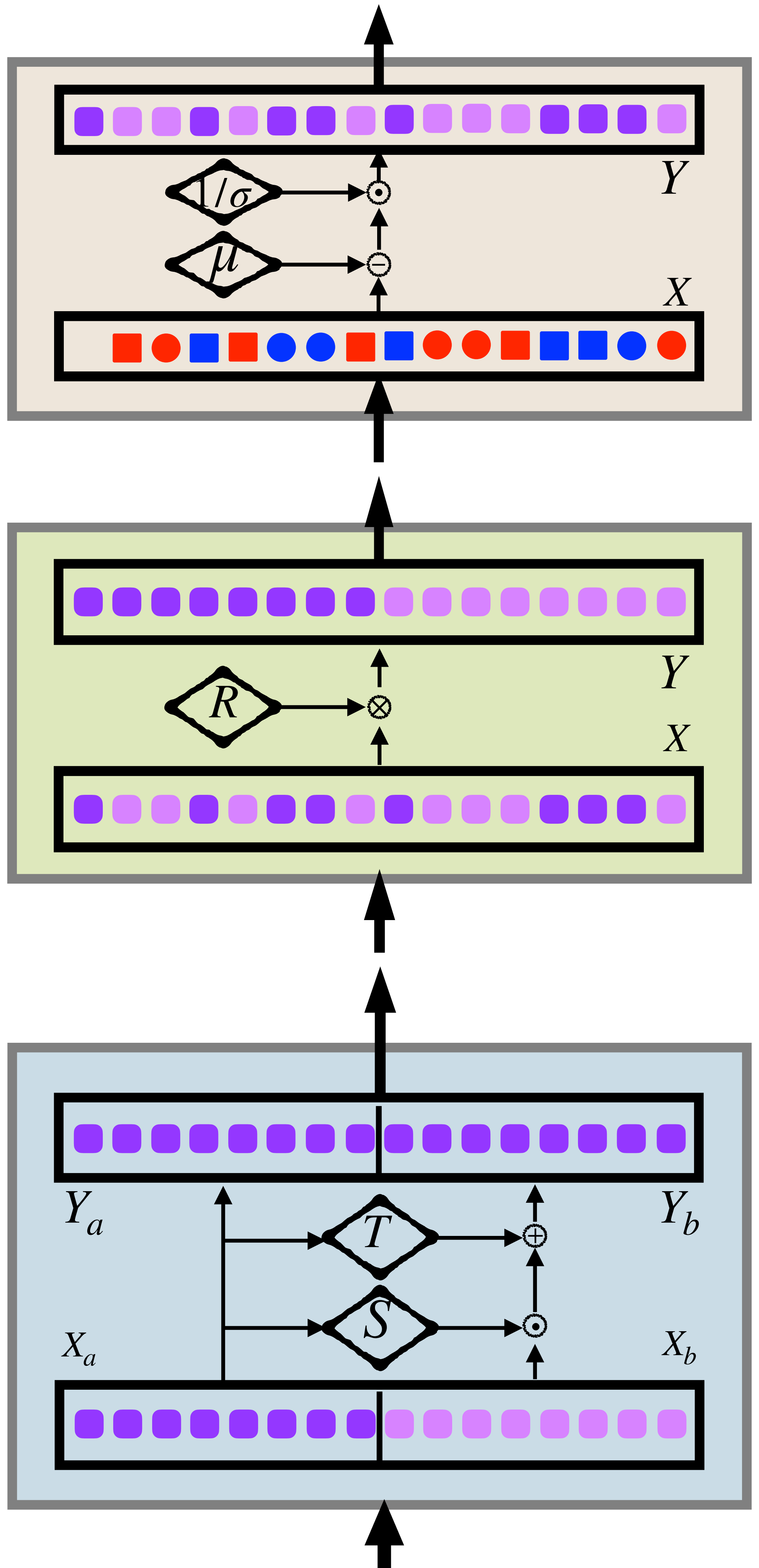
$$Y = R \times X$$

Affine Coupling

$$S, T = \text{NN}(X_a)$$

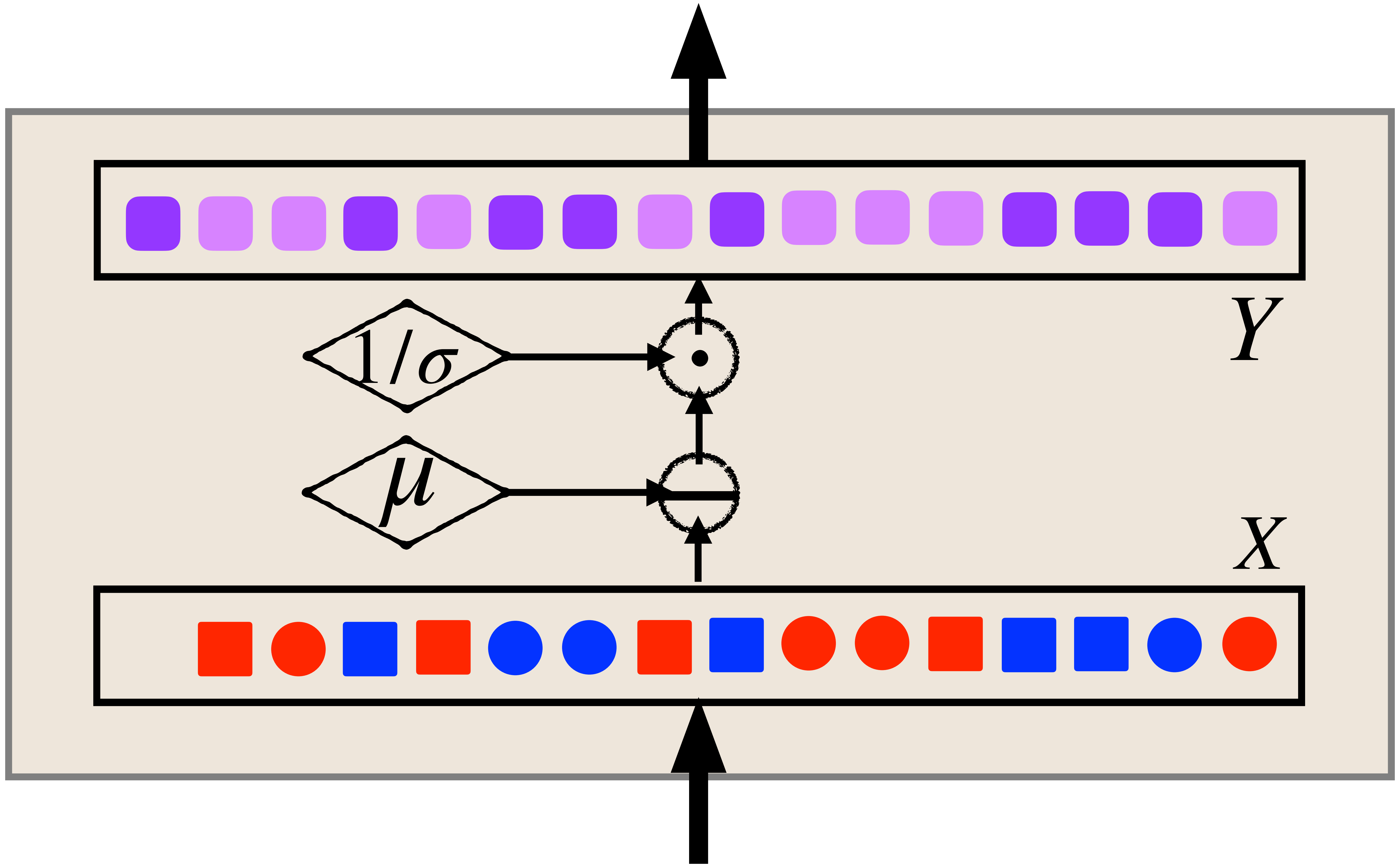
$$Y_b = S \odot X_b + T$$

$$Y_a = X_a$$



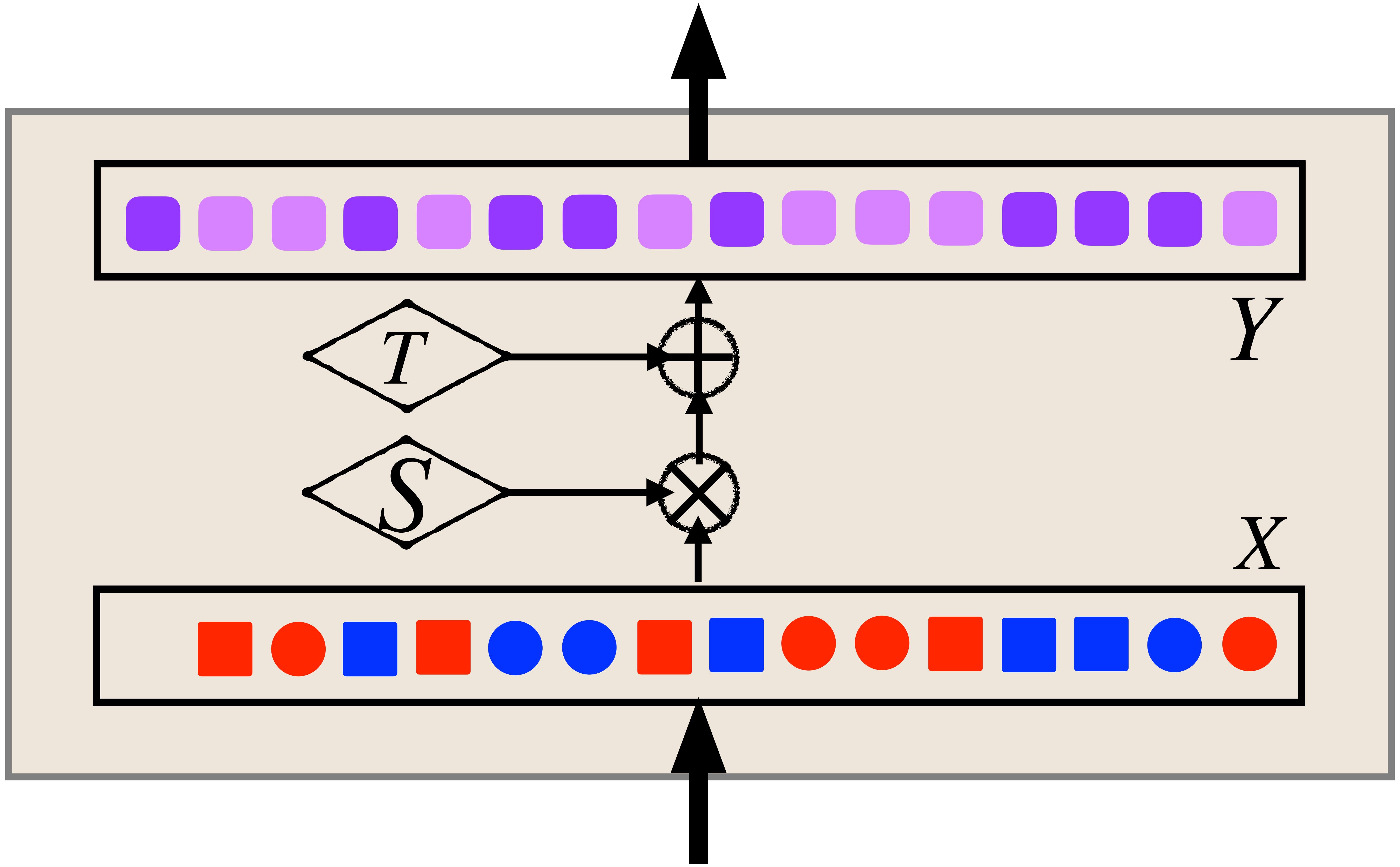
Actnorm

$$Y = \frac{1}{\sigma} \odot (X - \mu)$$



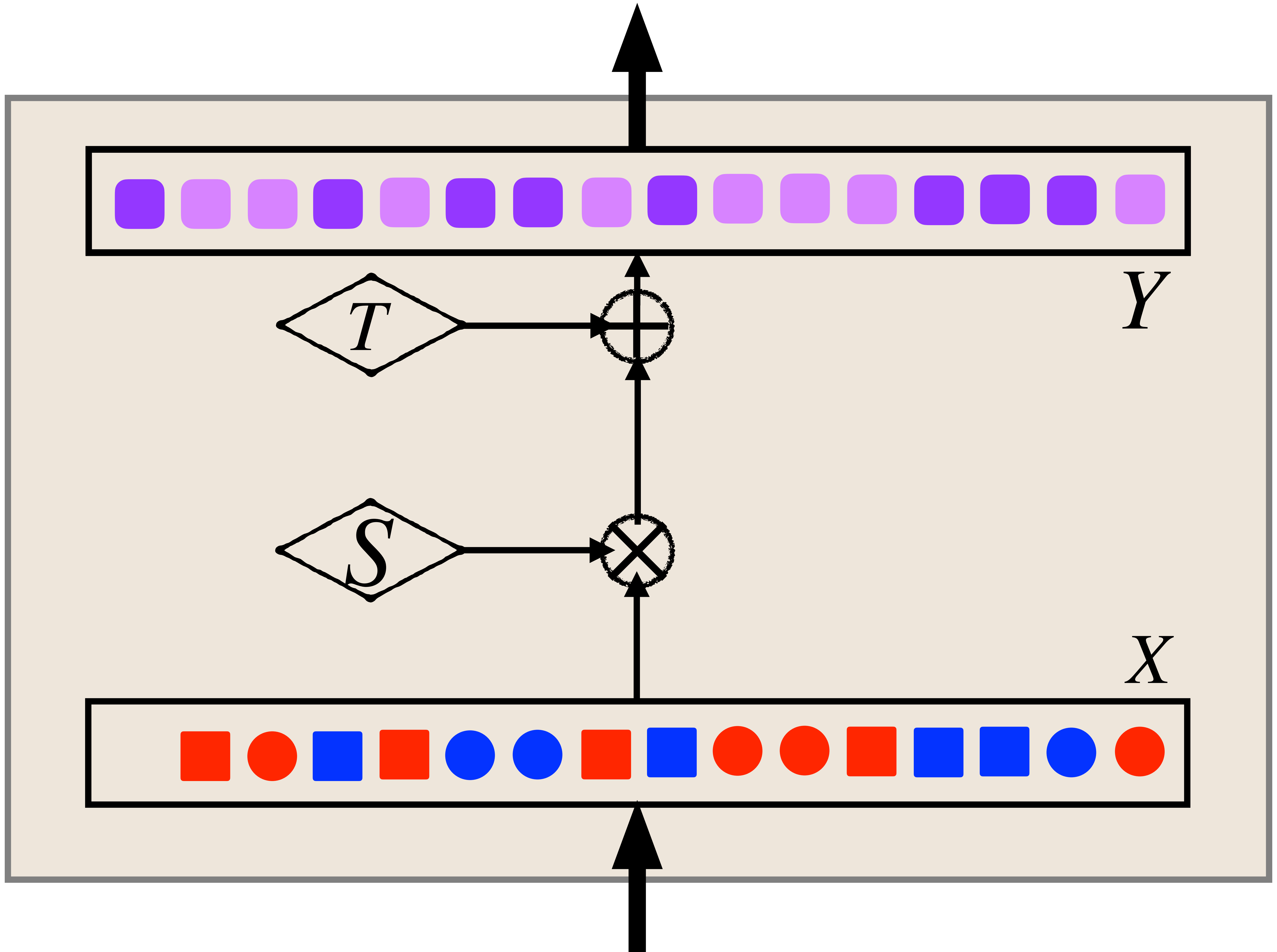
Actnorm

$$Y = \frac{1}{\sigma} \odot (X - \mu) \; = S \times X + T$$



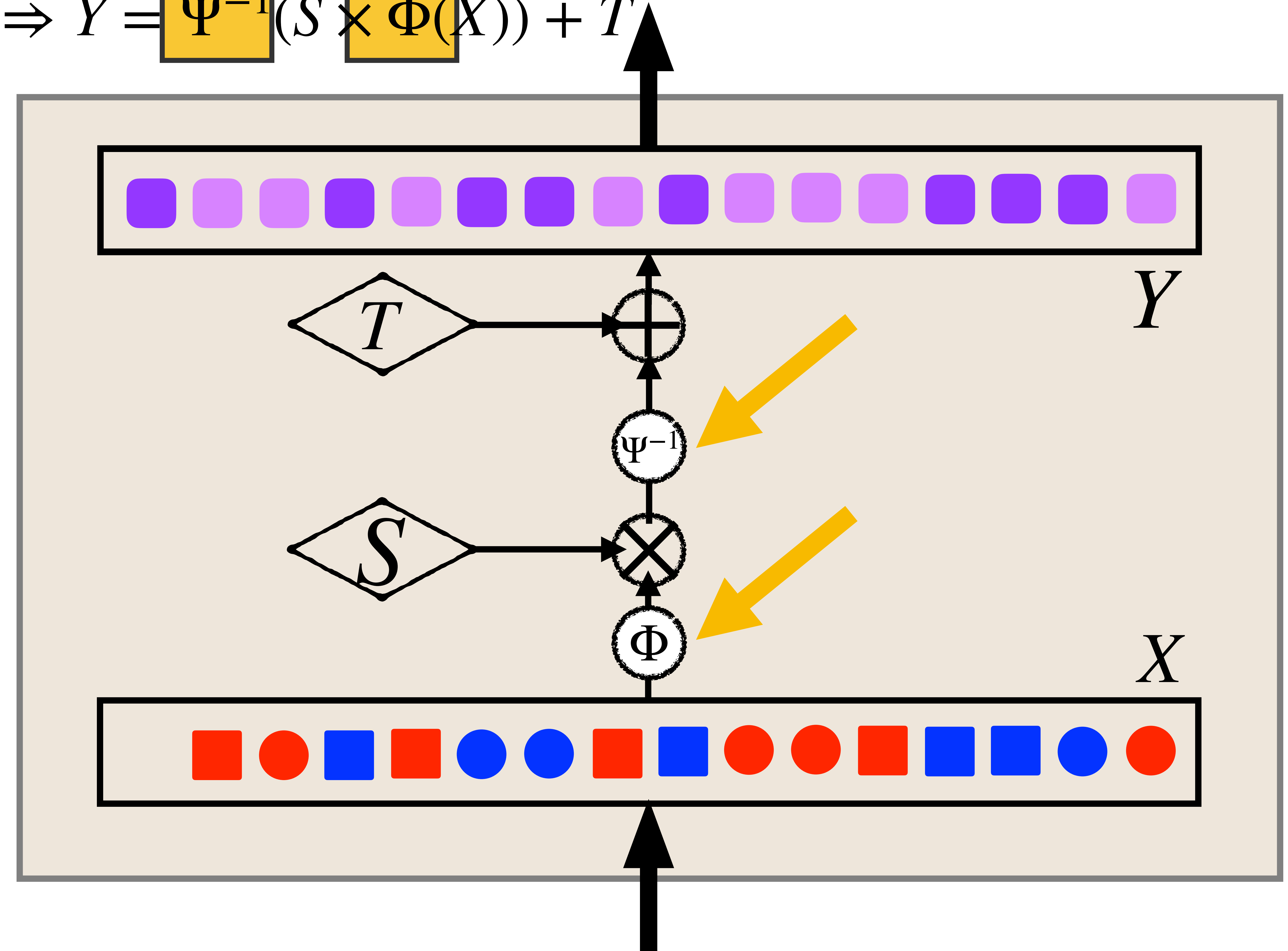
Actnorm

$Y = S \times X + T$



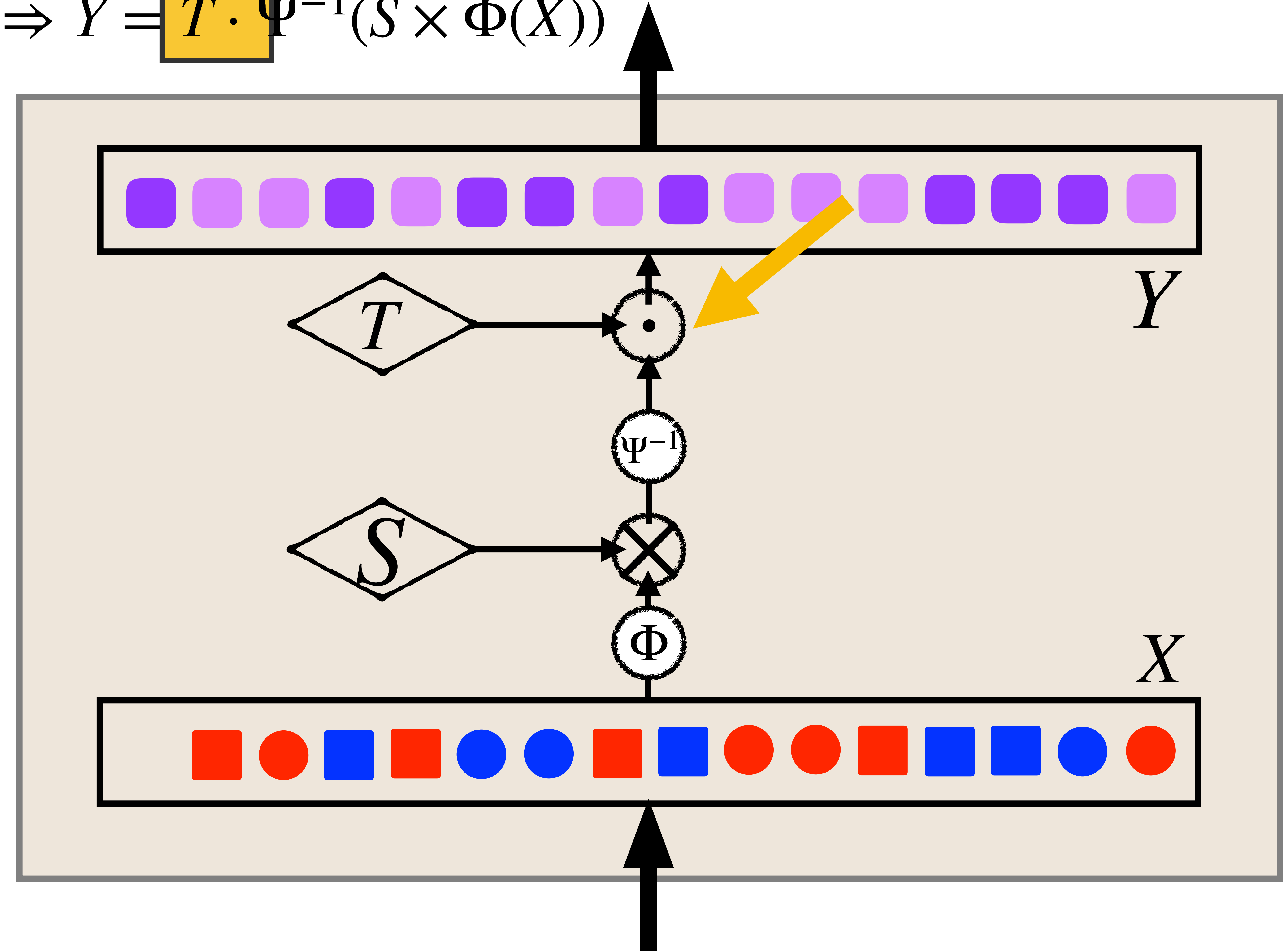
Actnorm

$$Y = S \times X + T \Rightarrow Y = \boxed{\Psi^{-1}}(S \times \boxed{\Phi}(X)) + T$$



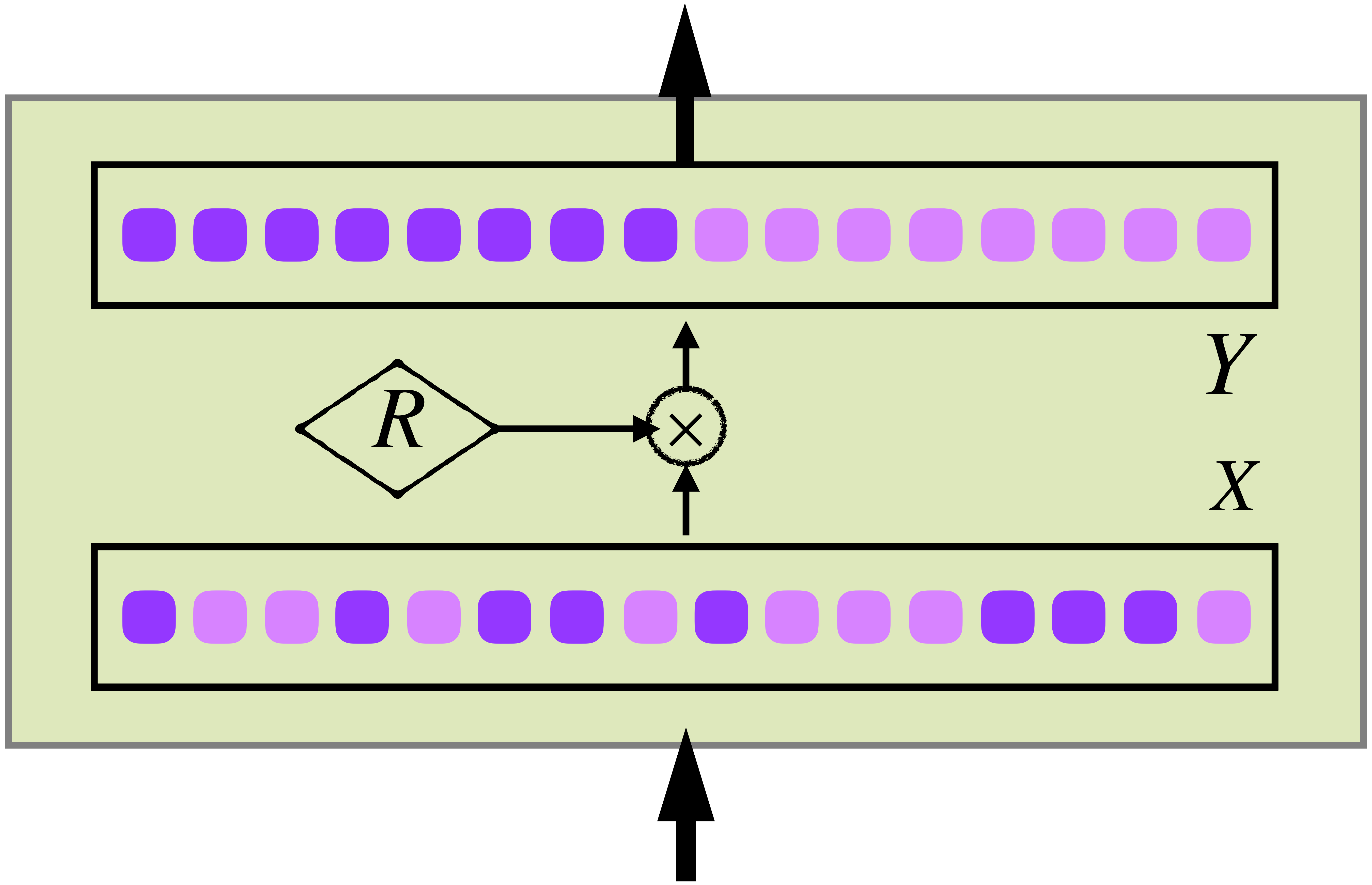
Actnorm

$$Y = S \times X + T \Rightarrow Y = \boxed{T \cdot} \Psi^{-1}(S \times \Phi(X))$$



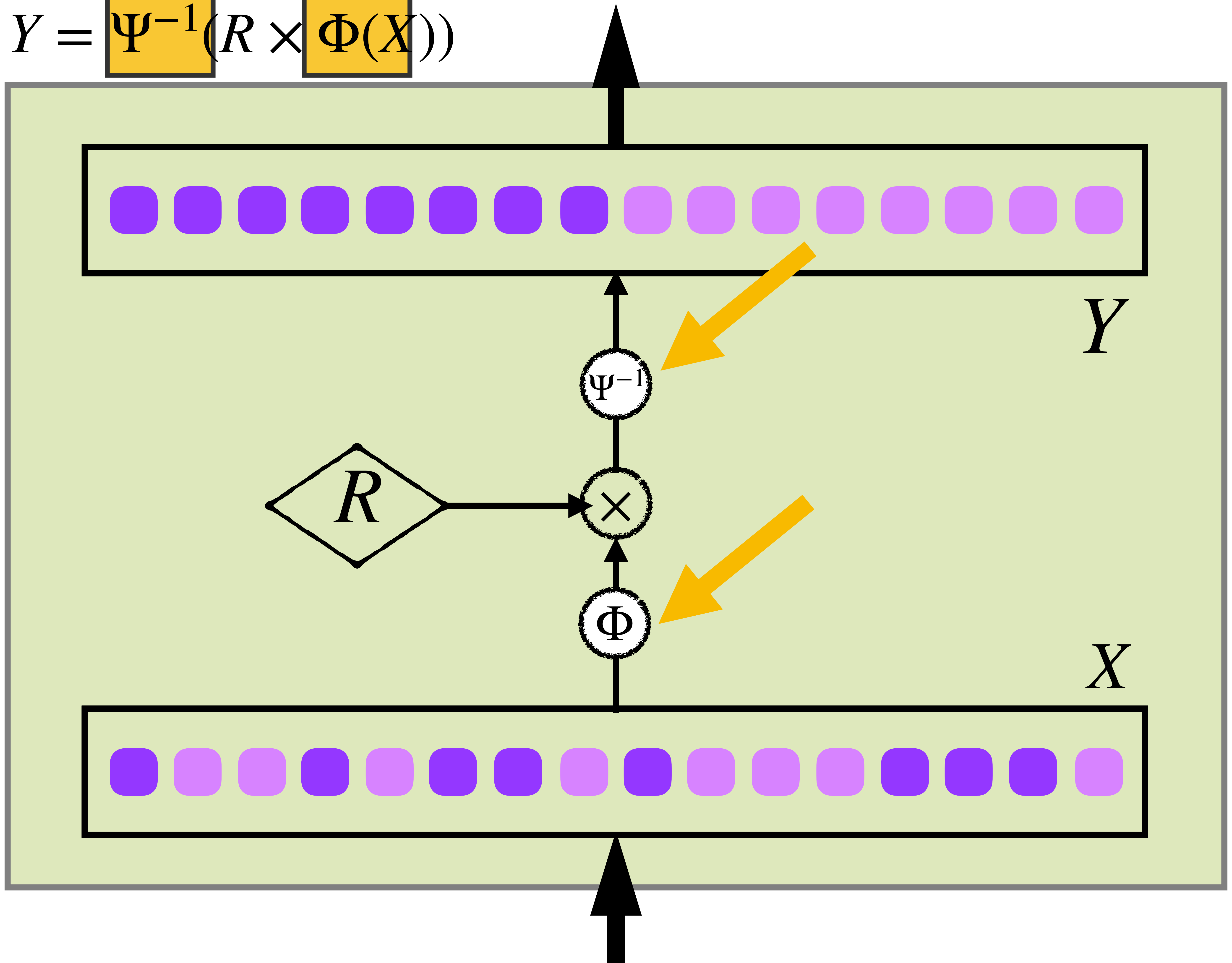
1×1 convolution

$Y = \boxed{R \times} X$



1×1 convolution

$Y = R \times X \quad \Rightarrow Y = \boxed{\Psi^{-1}}(R \times \boxed{\Phi(X)})$

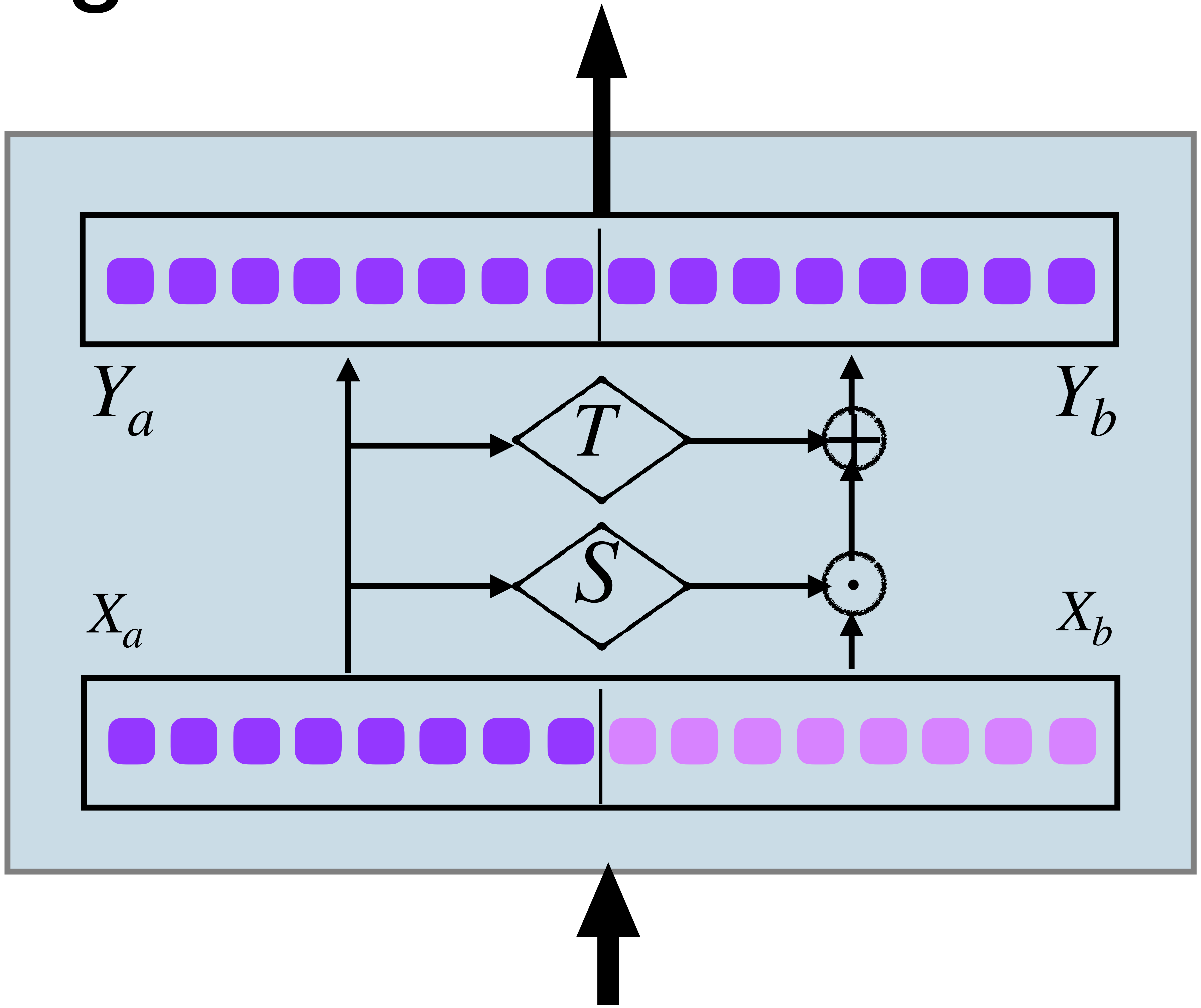


Affine Coupling

$S, T = \boxed{\text{NN}}(X_a)$

$Y_b = S \odot X_b + T$

$Y_a = X_a$

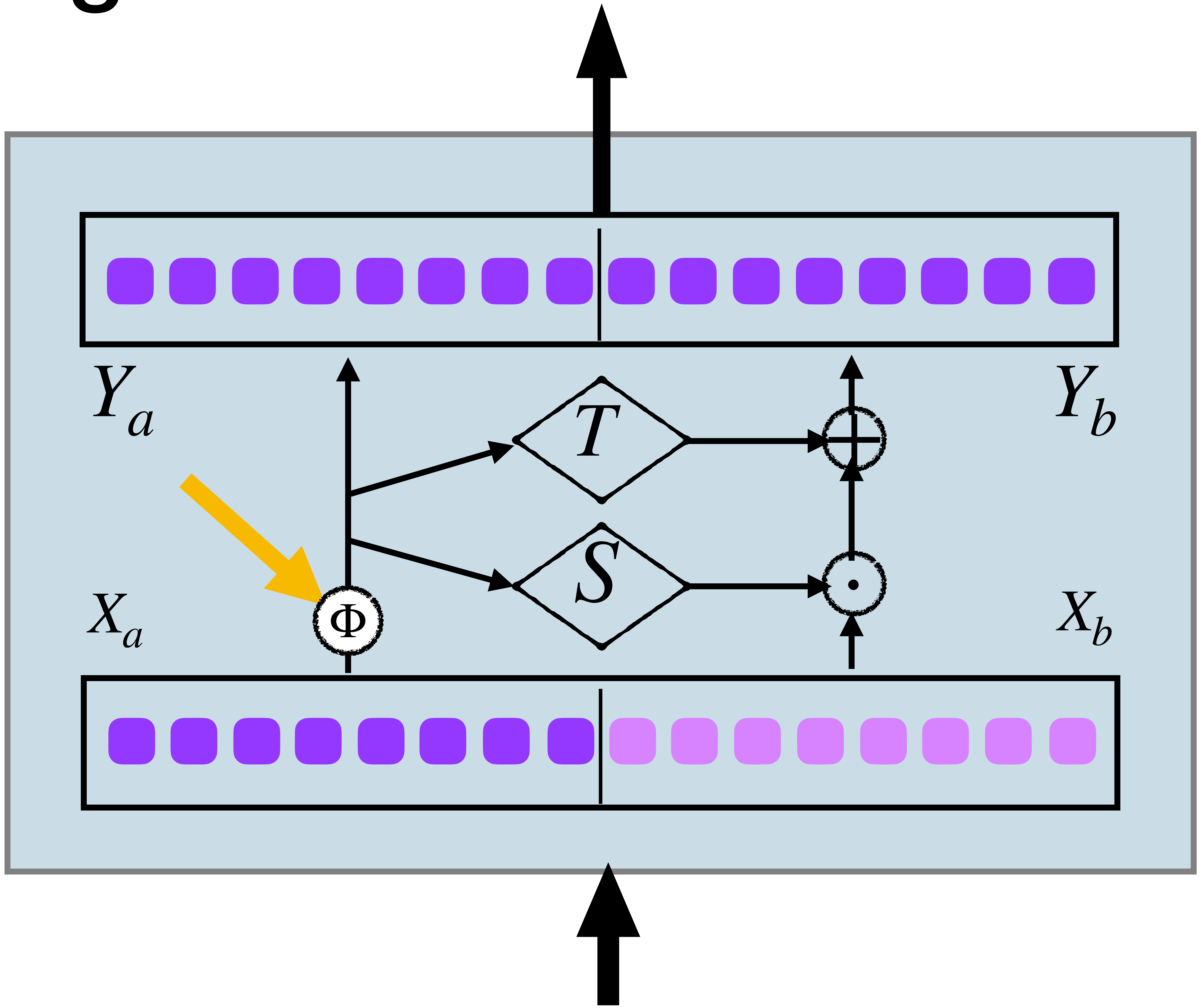


Affine Coupling

$S, T = \boxed{\mathrm{NN}}(\Phi(X_a))$

$Y_b = S \odot X_b + T$

$Y_a = X_a$

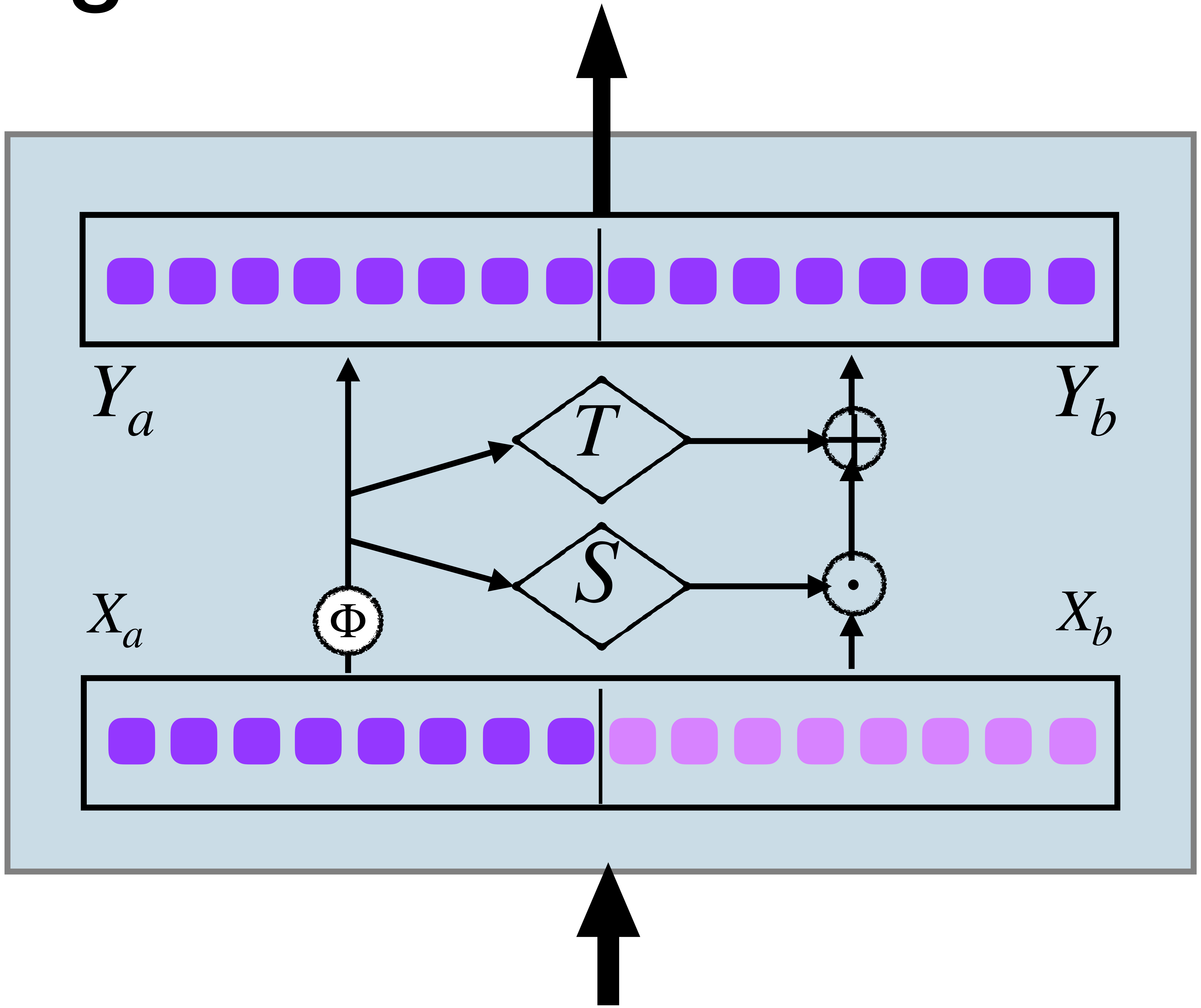


Affine Coupling

$S, T = \boxed{\text{NN}}(\Phi(X_a))$

$Y_b = \boxed{S \odot} X_b \boxed{+ T}$

$Y_a = X_a$

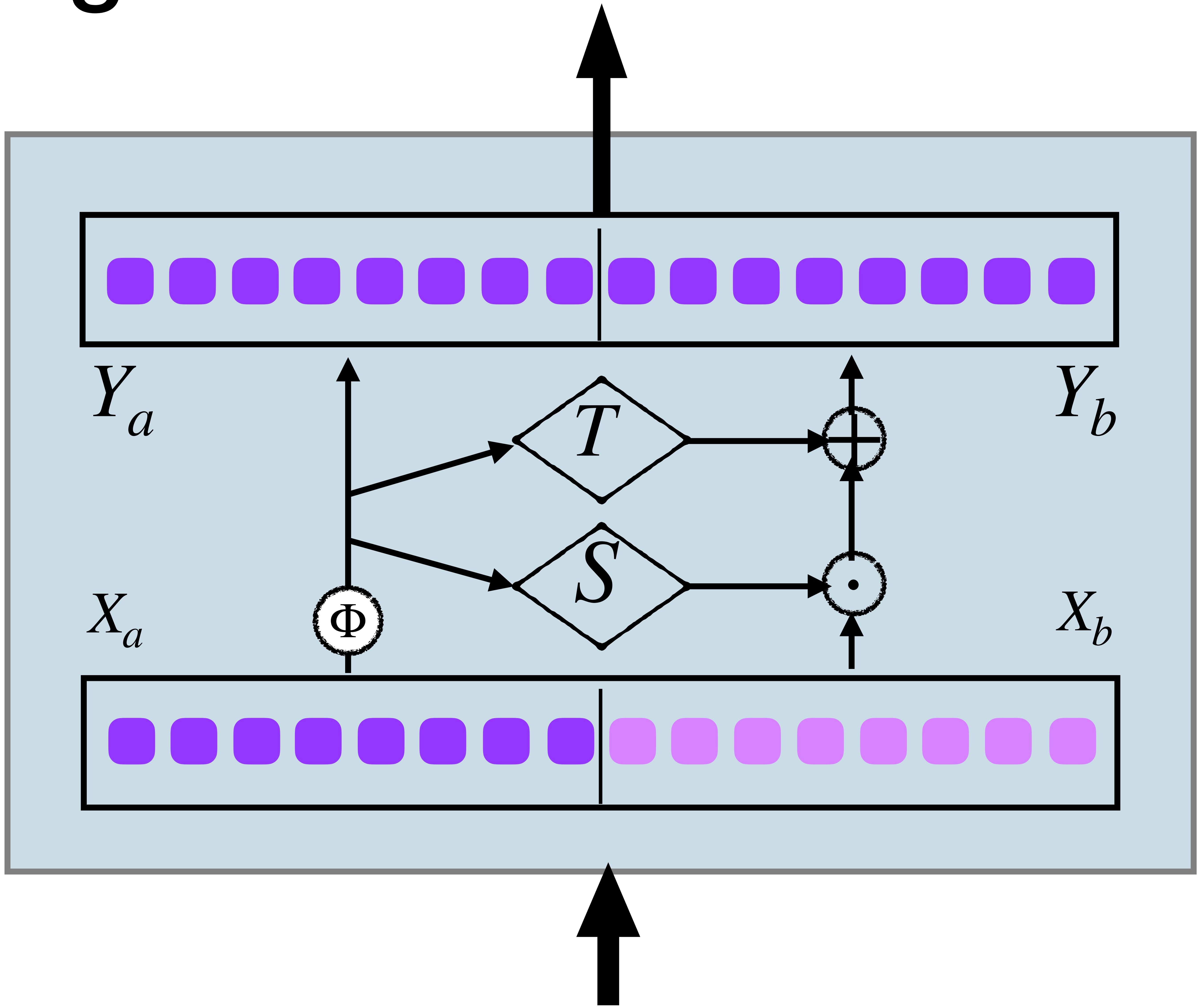


Affine Coupling

$S, T = \boxed{\mathrm{NN}}(\Phi(X_a))$

$Y_b = \boxed{T \cdot}(\boxed{S \times}\Phi(X_b))$

$Y_a = X_a$



Affine Coupling

$$S, T = \boxed{\mathrm{NN}}(\Phi(X_a))$$

$$Y_b = \boxed{T \cdot}(\boxed{S \times}\Phi(X_b))$$

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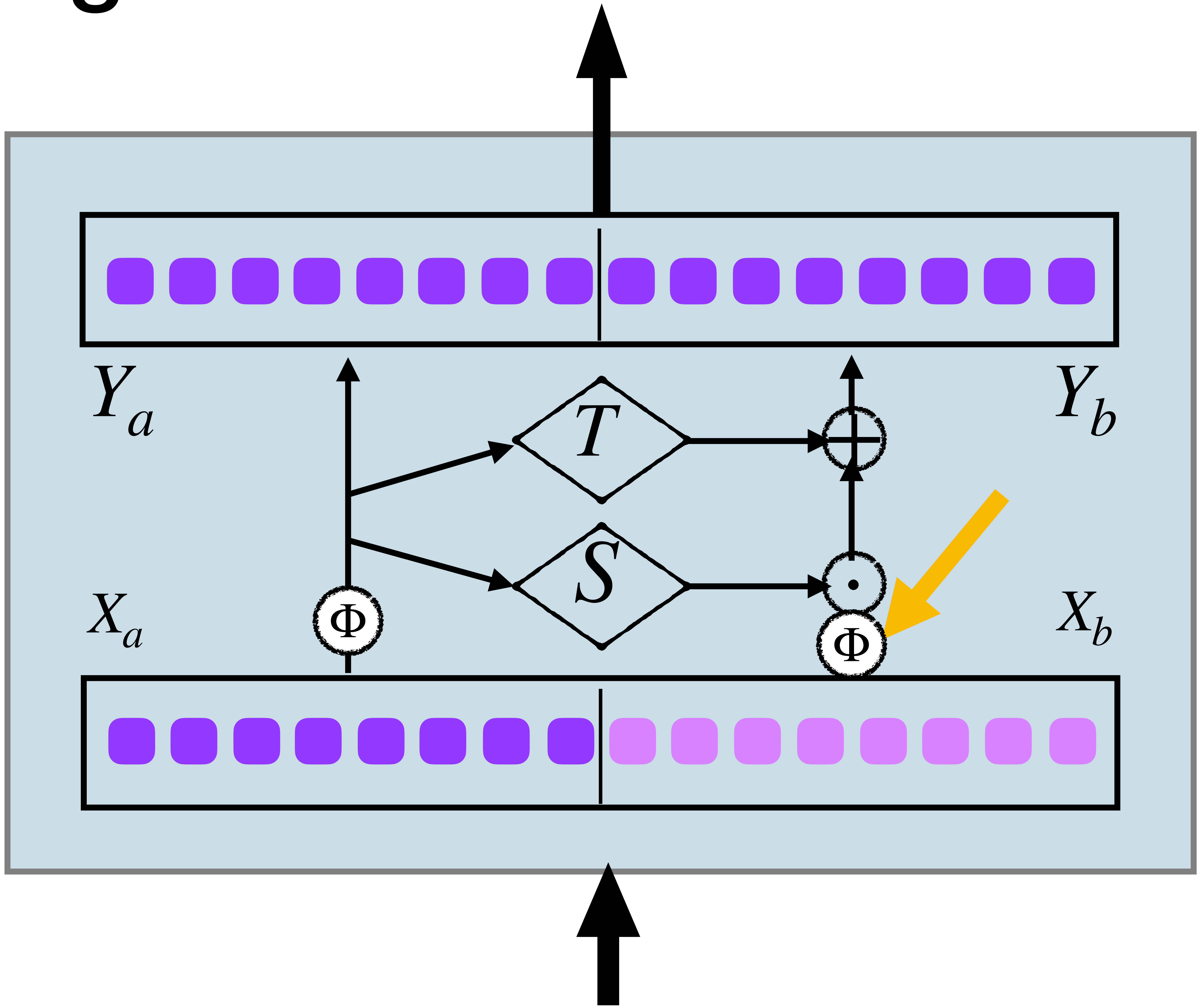
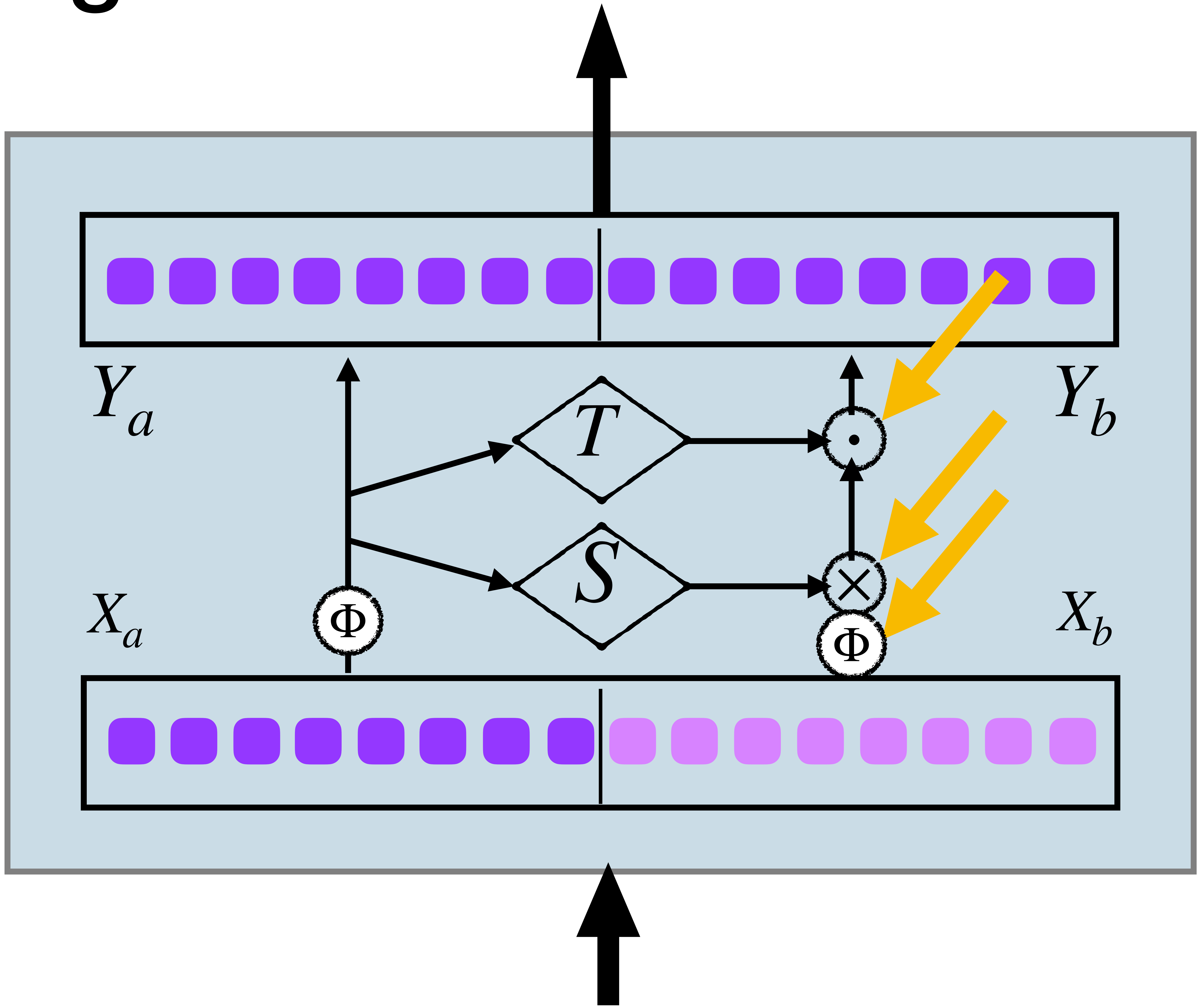


Affine Coupling

$$S, T = \boxed{\mathrm{NN}}(\Phi(X_a))$$

$$Y_b = \boxed{T \cdot}(\boxed{S \times}\Phi(X_b))$$

$$Y_a = X_a$$

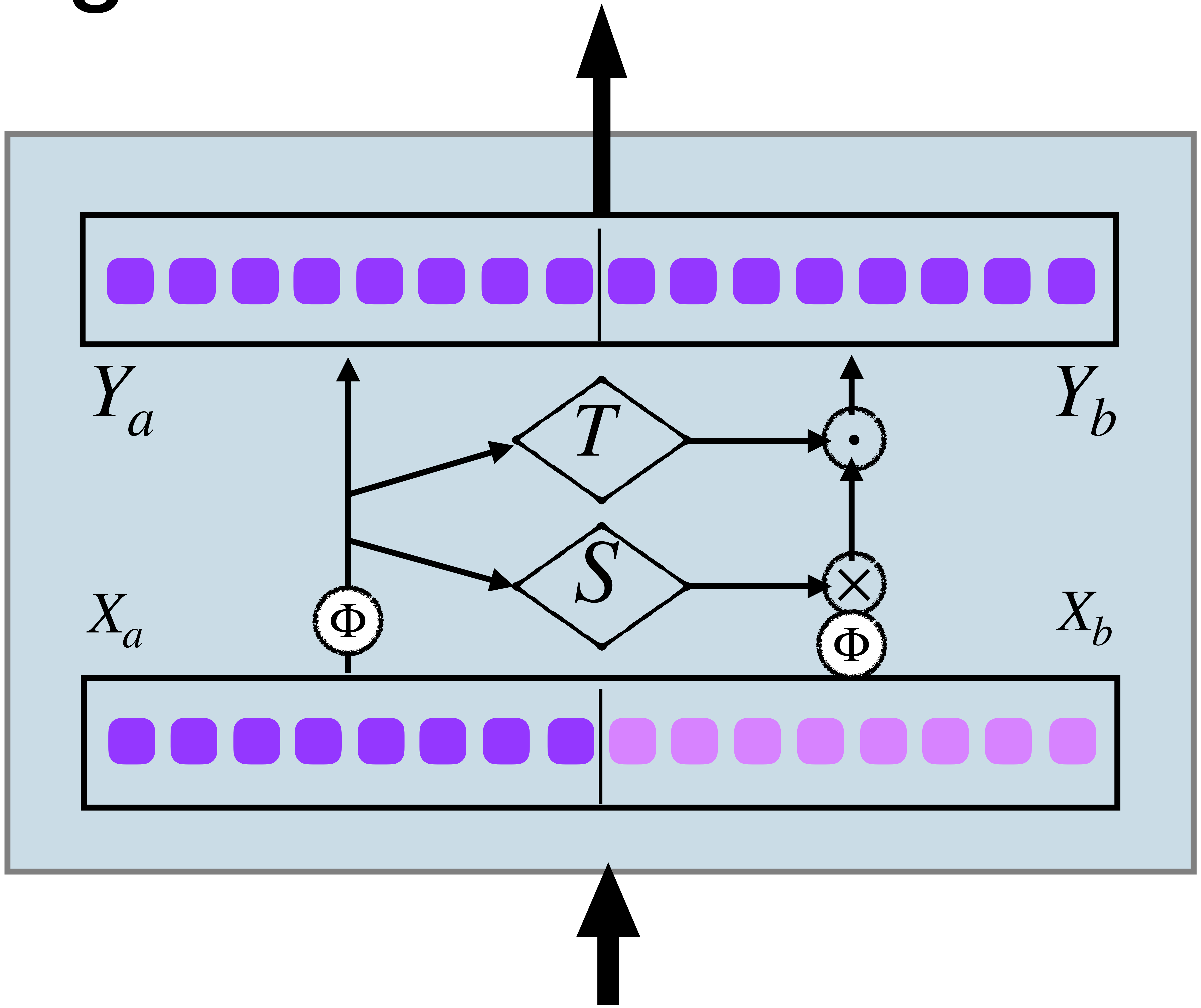


Affine Coupling

$S, T = \boxed{\mathrm{NN}(}\Phi(X_a))$

$Y_b = \boxed{T \cdot (}\boxed{S \times}\Phi(X_b))$

$Y_a = \boxed{X_a} = \Phi^{-1}(\Phi(X_a))$

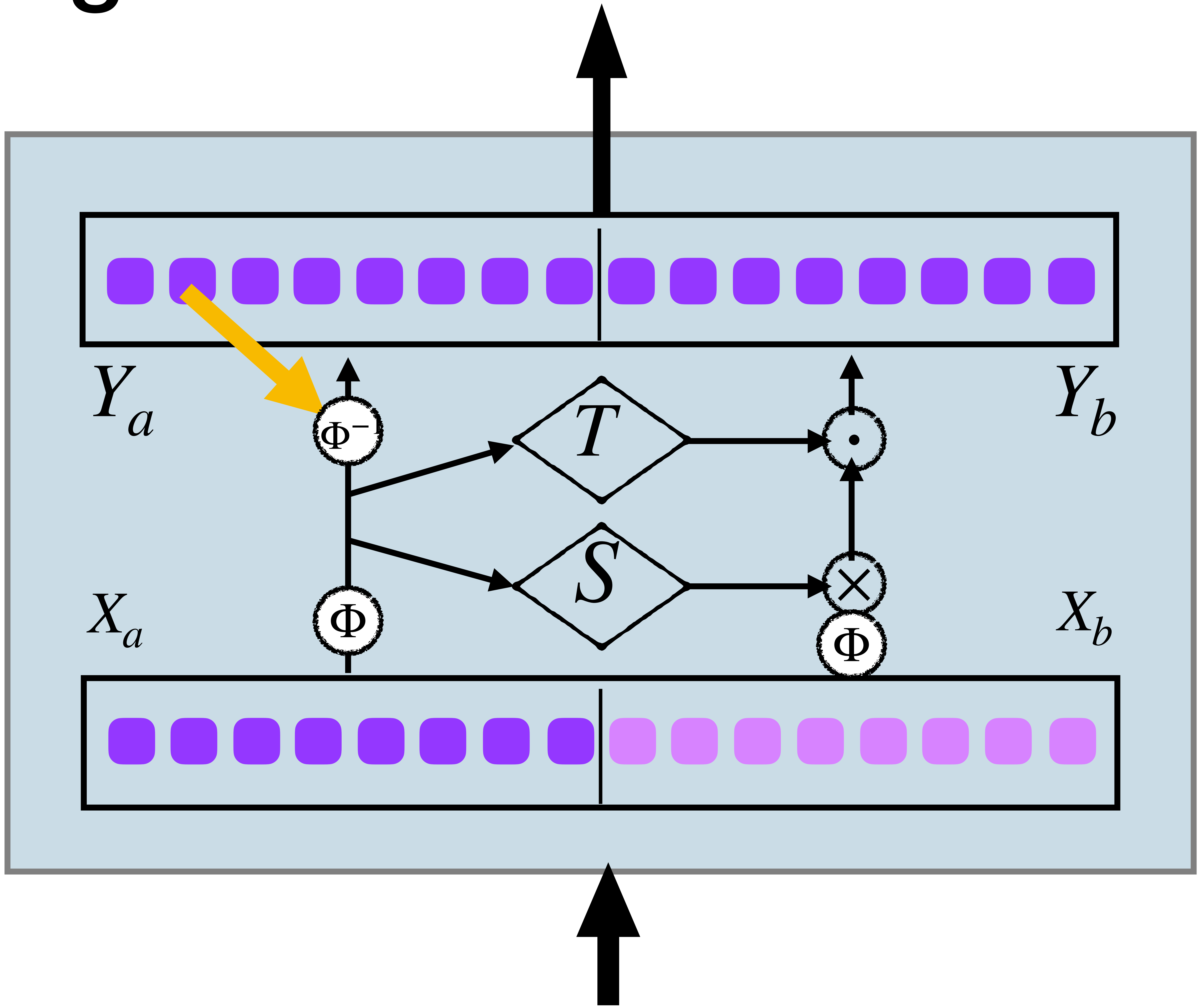


Affine Coupling

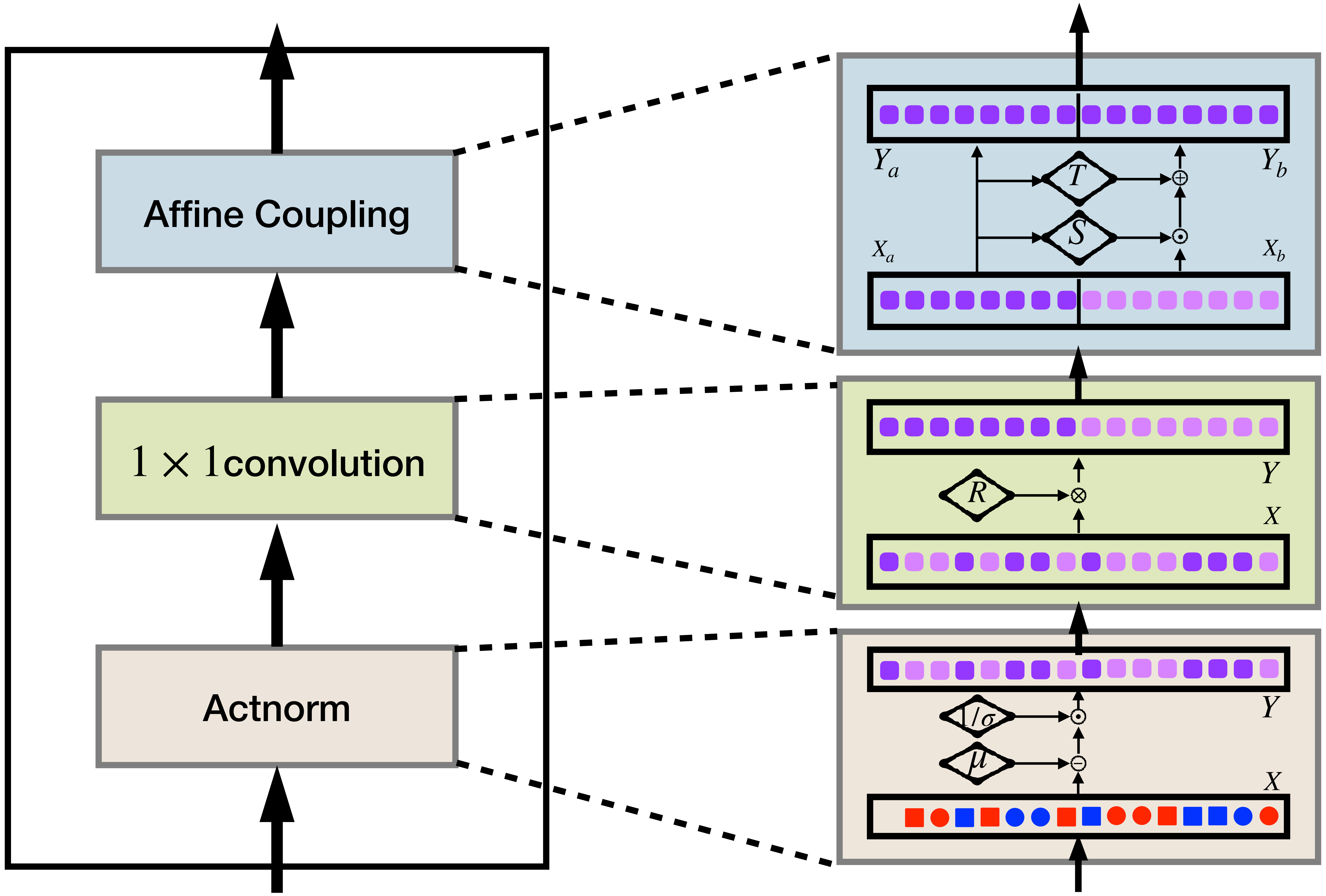
$$S, T = \mathrm{NN}(\Phi(X_a))$$

$$Y_b = T \cdot (S \times \Phi(X_b))$$

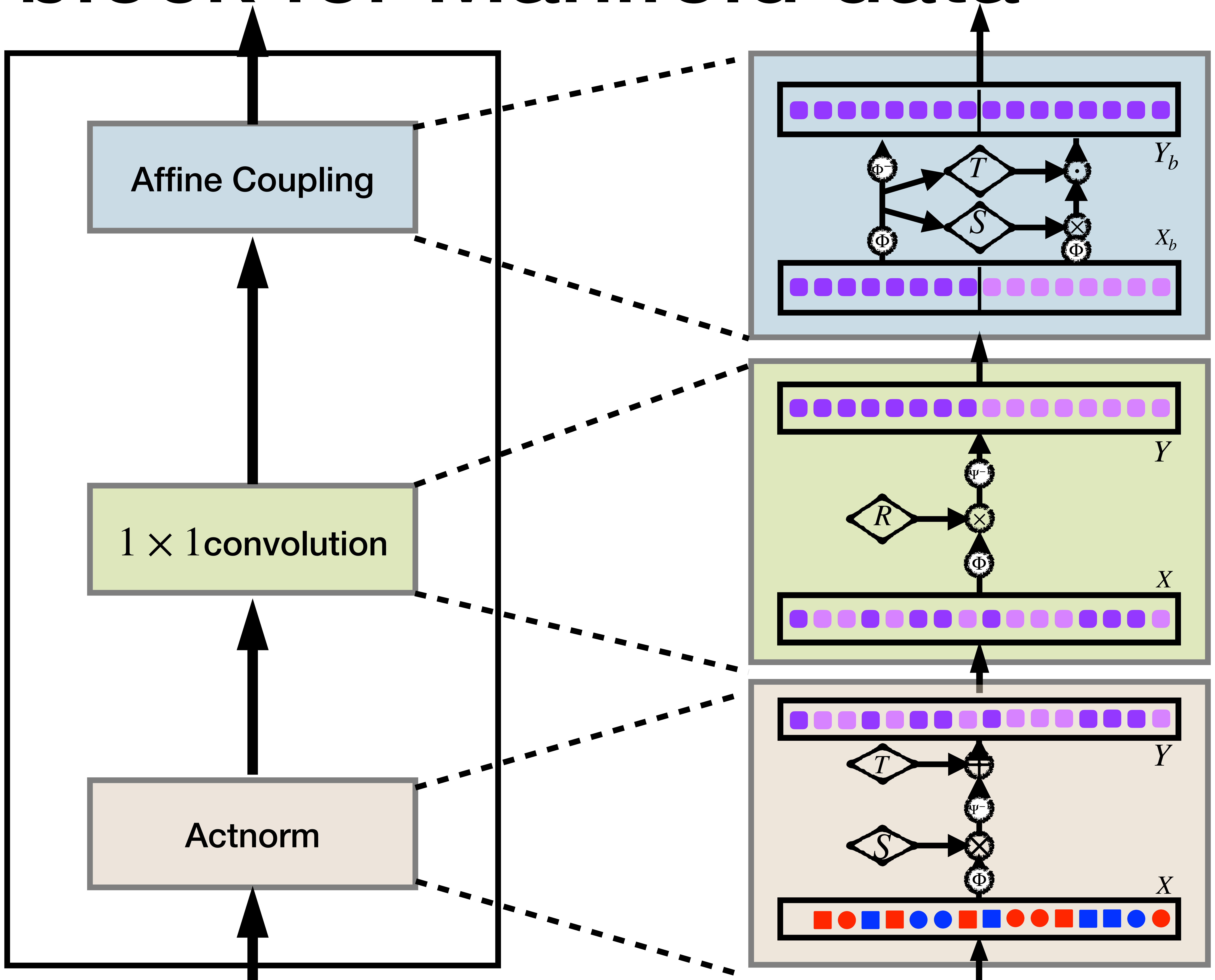
$$Y_a = X_a = \Phi^{-1}(\Phi(X_a))$$



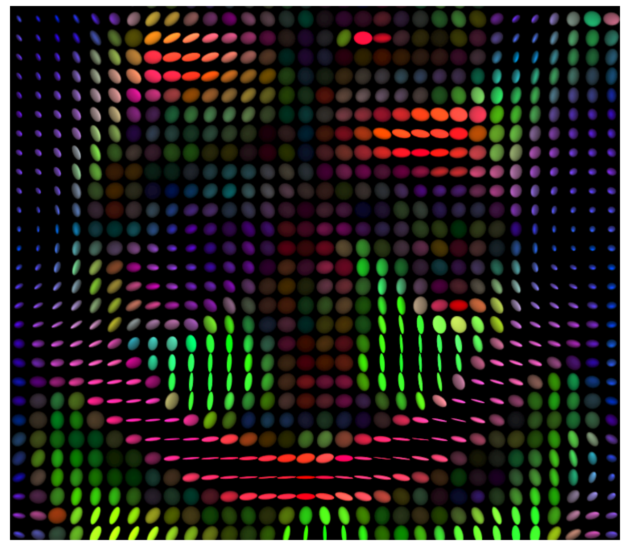
A basic block for Euclidean data



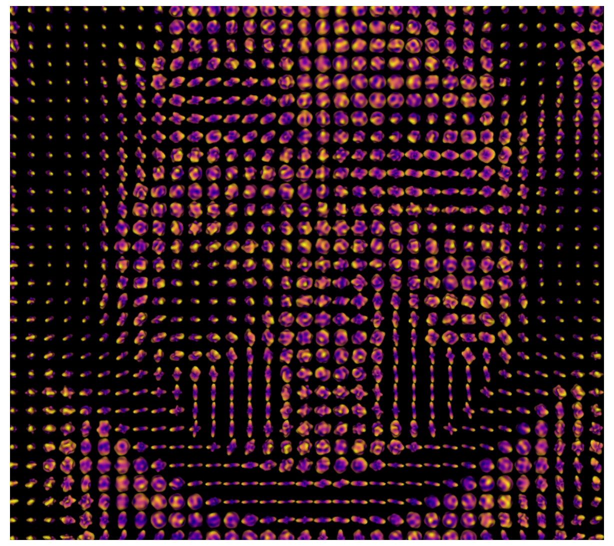
A basic block for Manifold data



From DTI to ODF

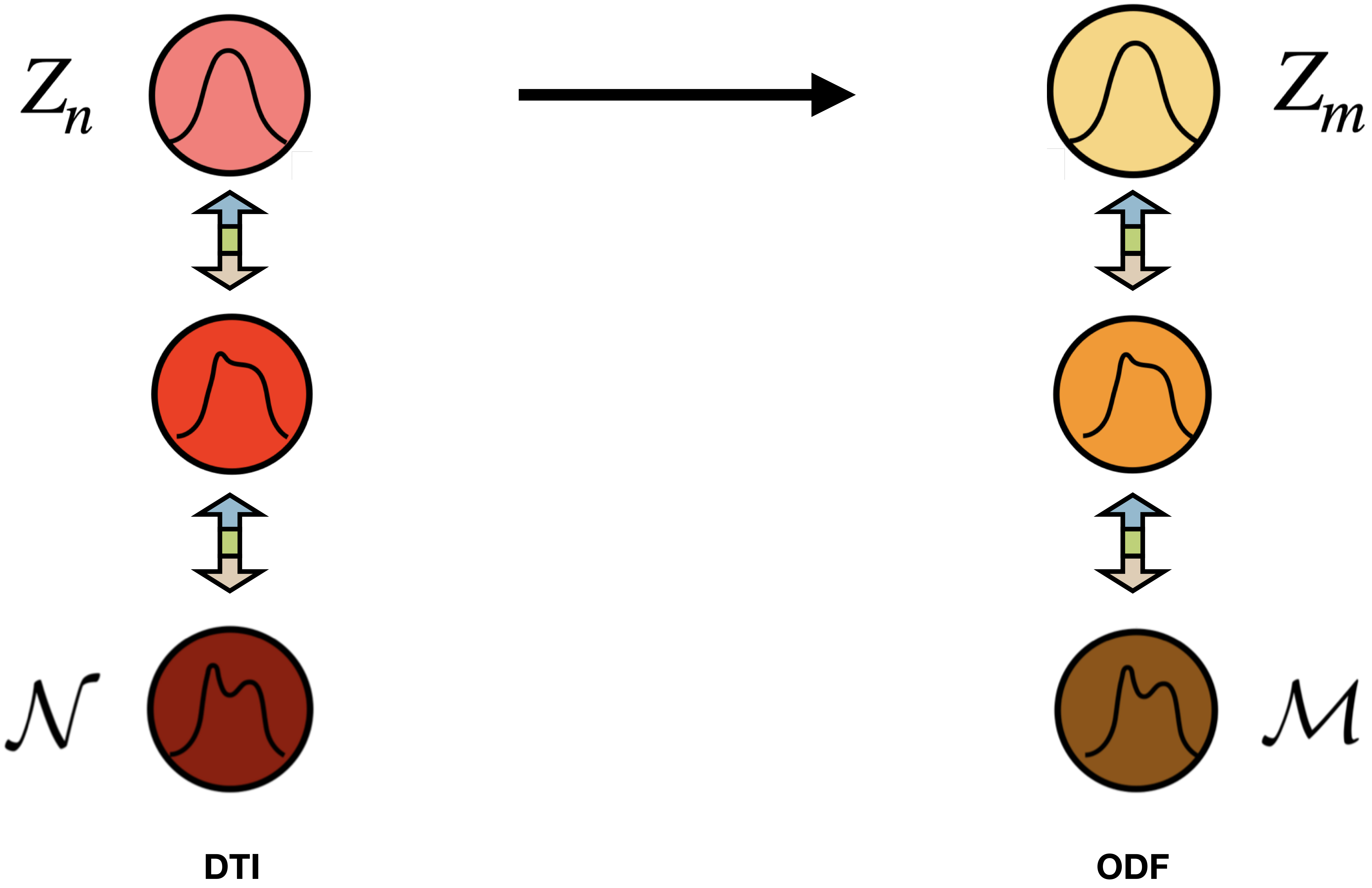


DTI



ODF

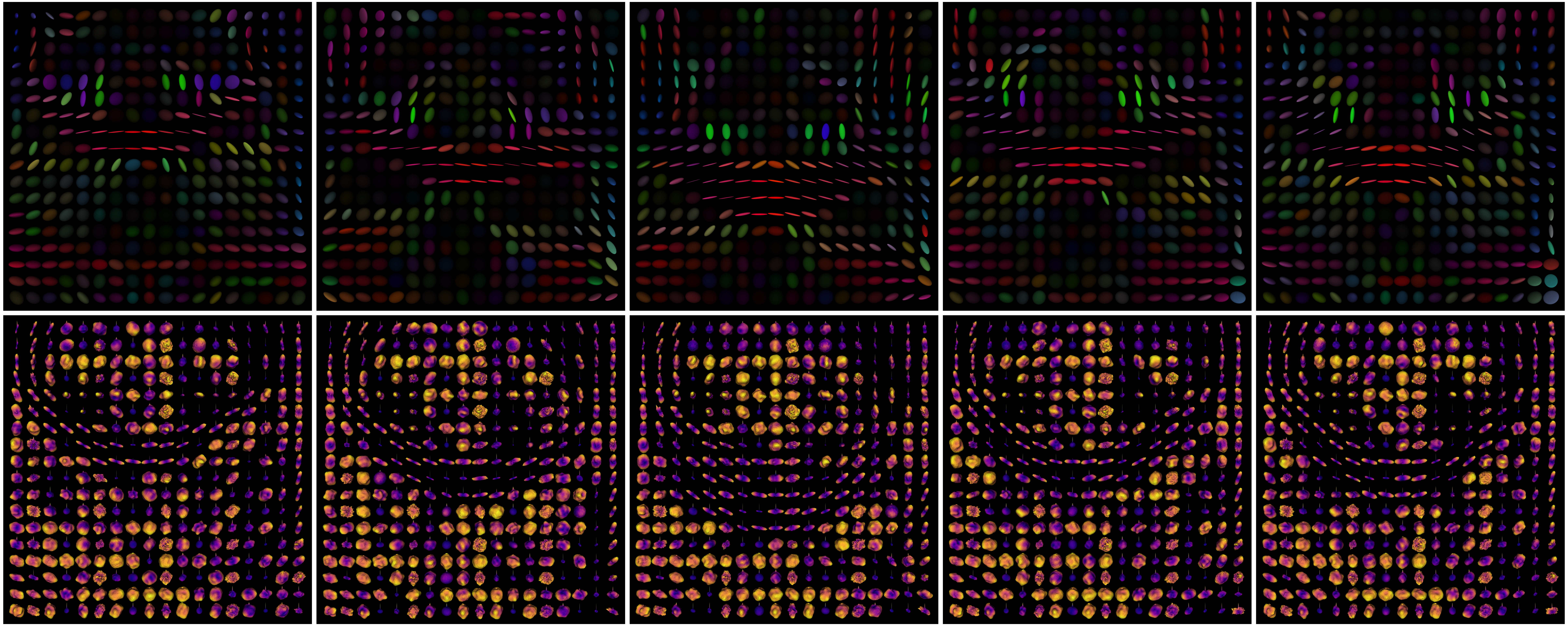
From DTI to ODF



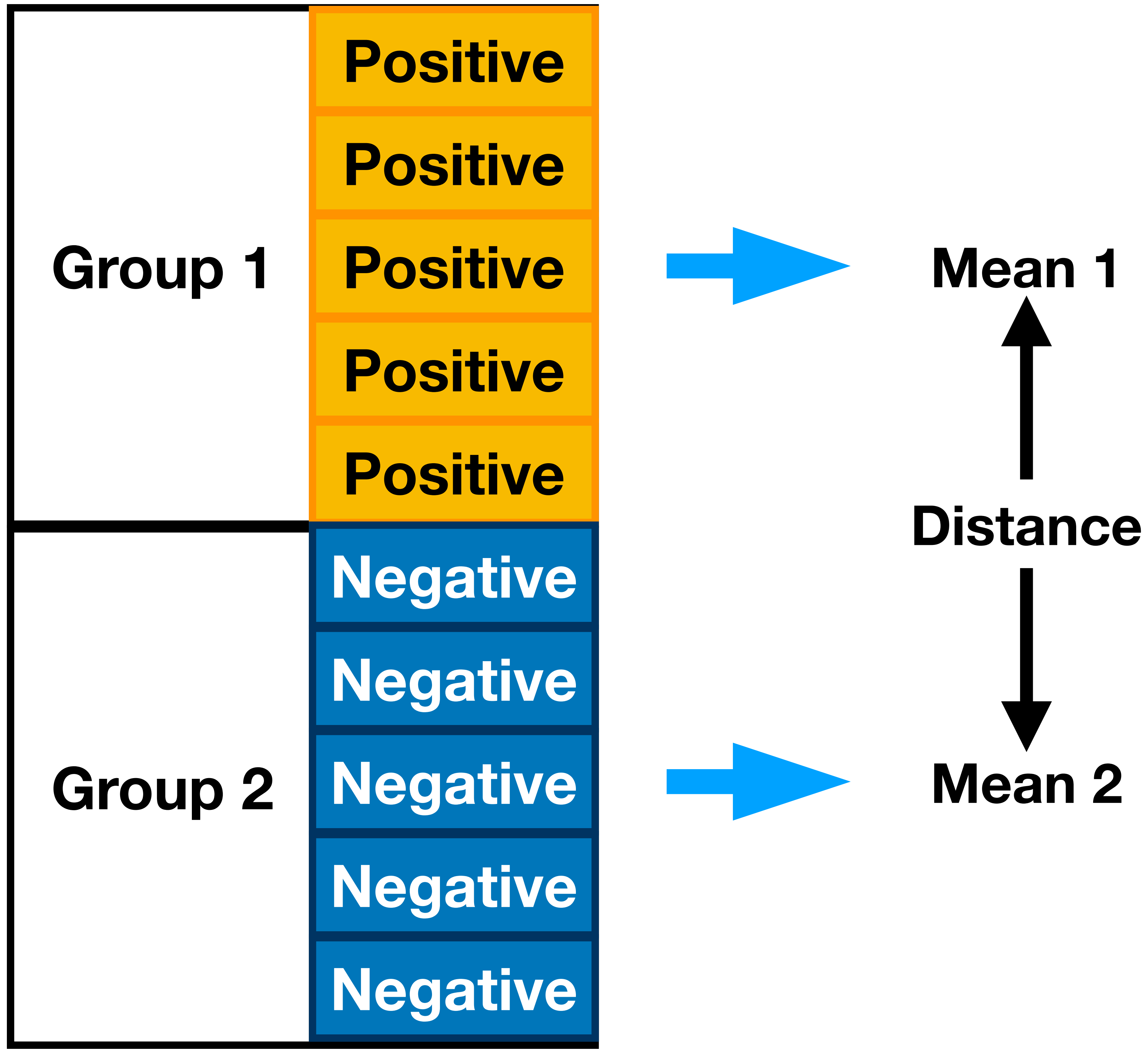
Experiment - HCP dataset

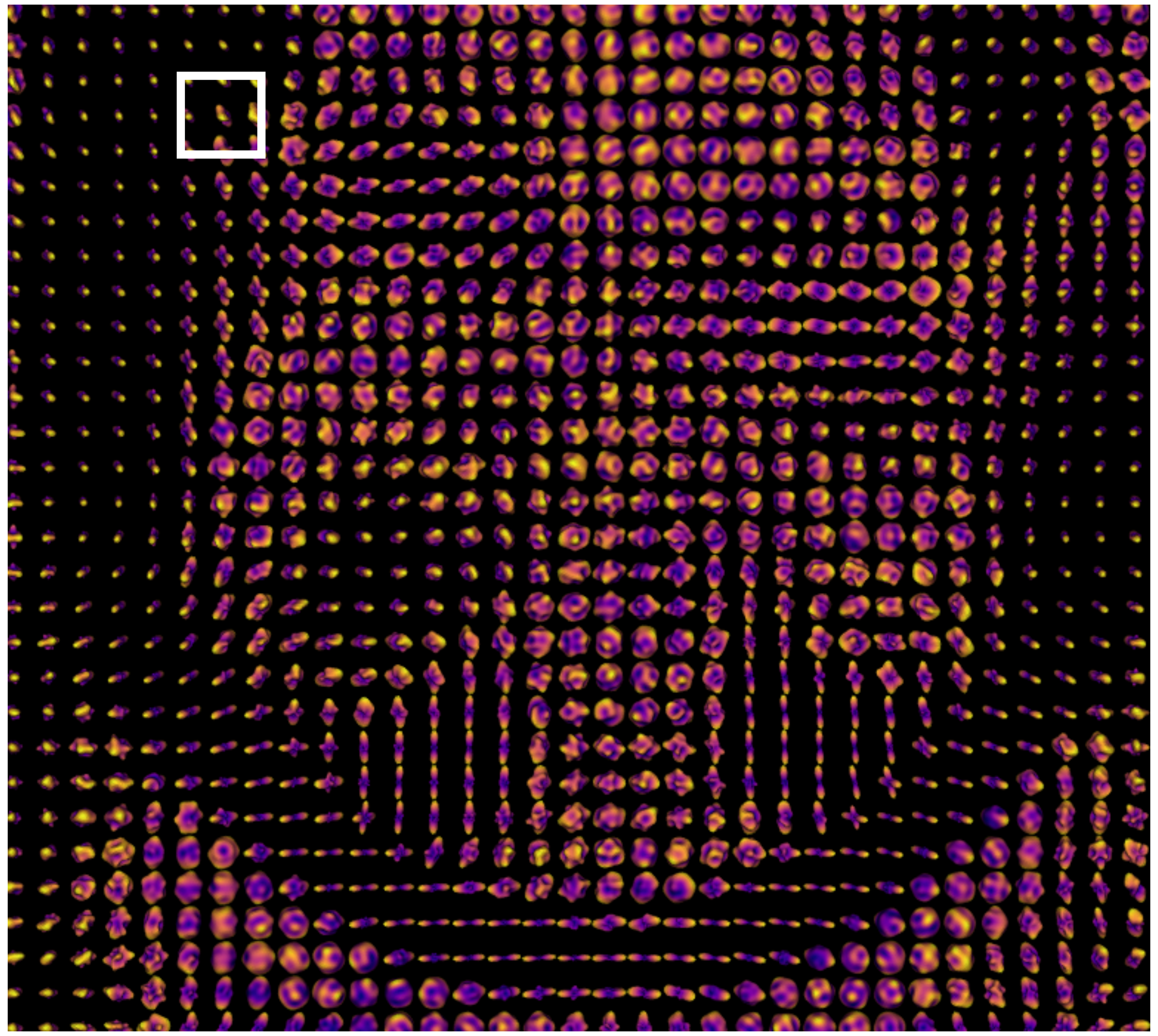
Figure by Joshi, etc. Figure by Hagmann, etc.

Experiment - Some generated examples

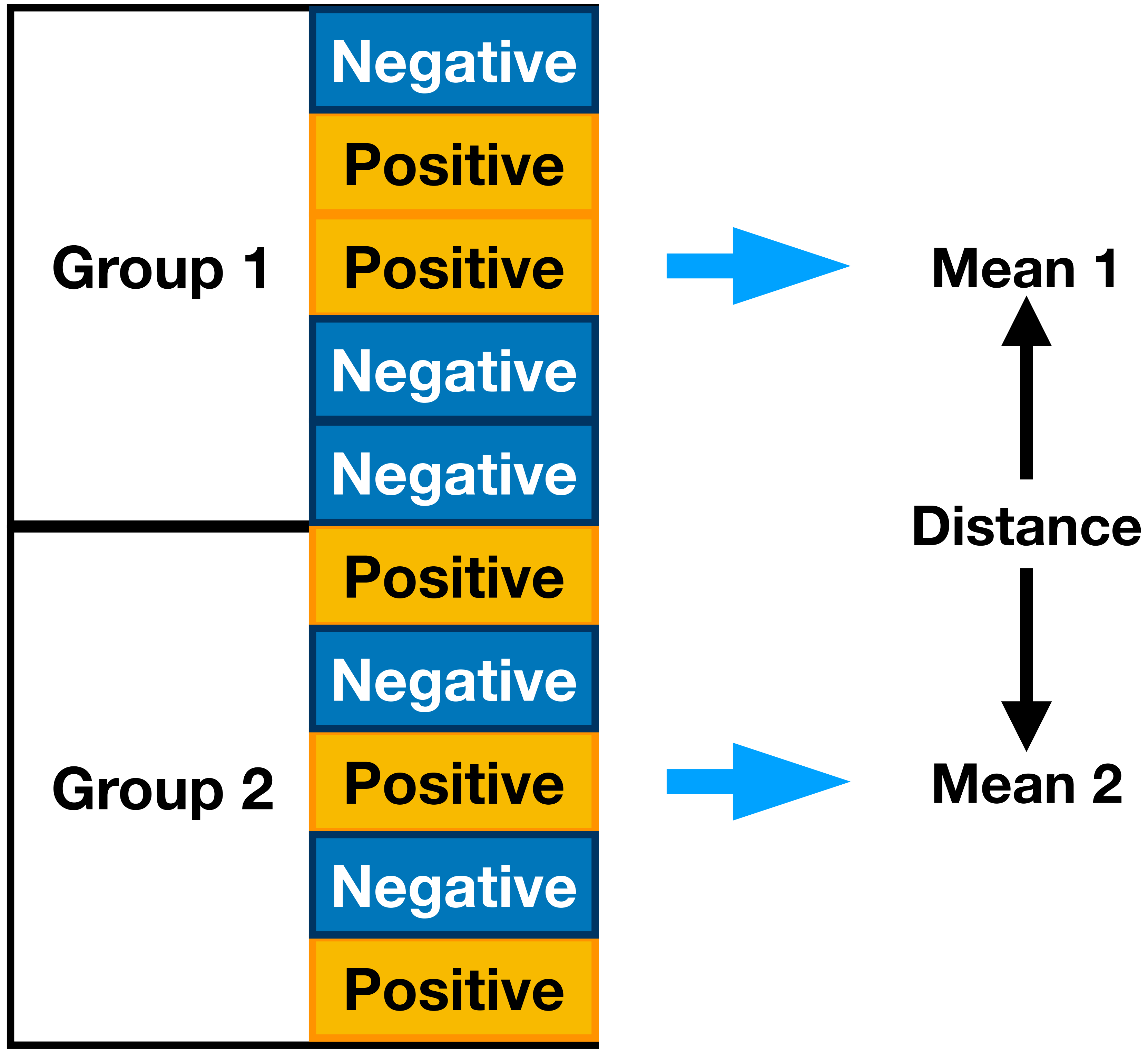


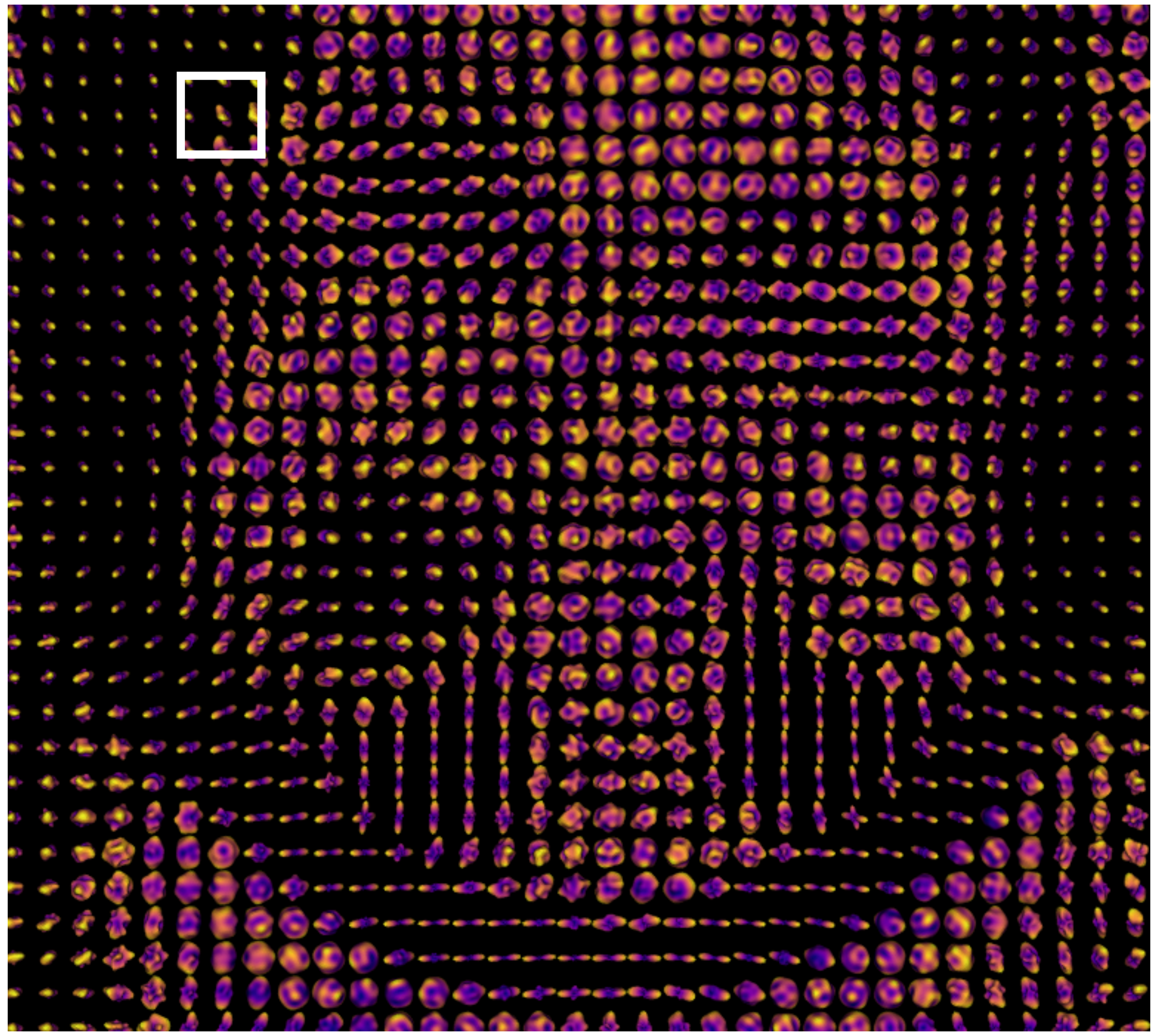
Experiment - Group difference analysis



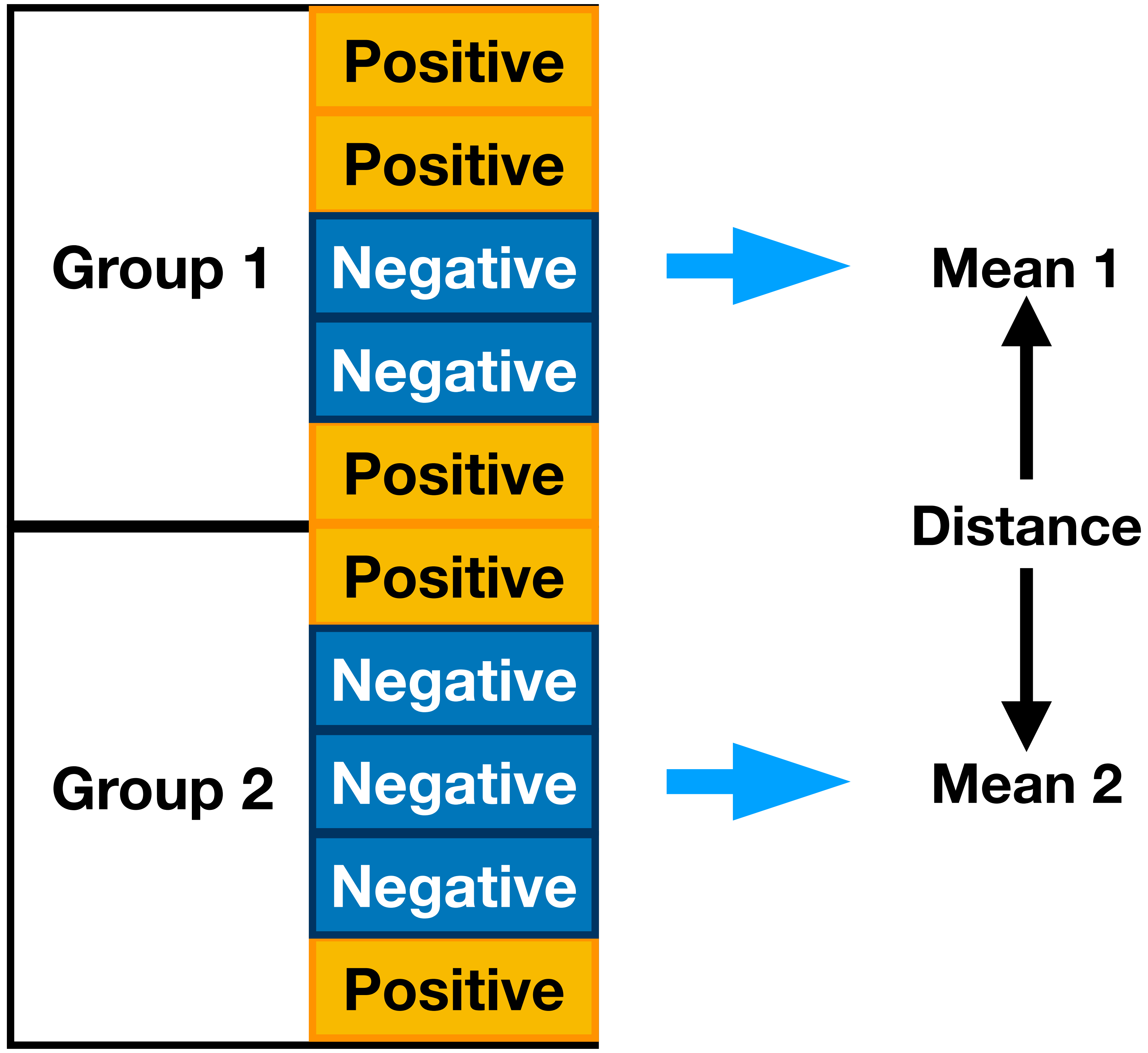


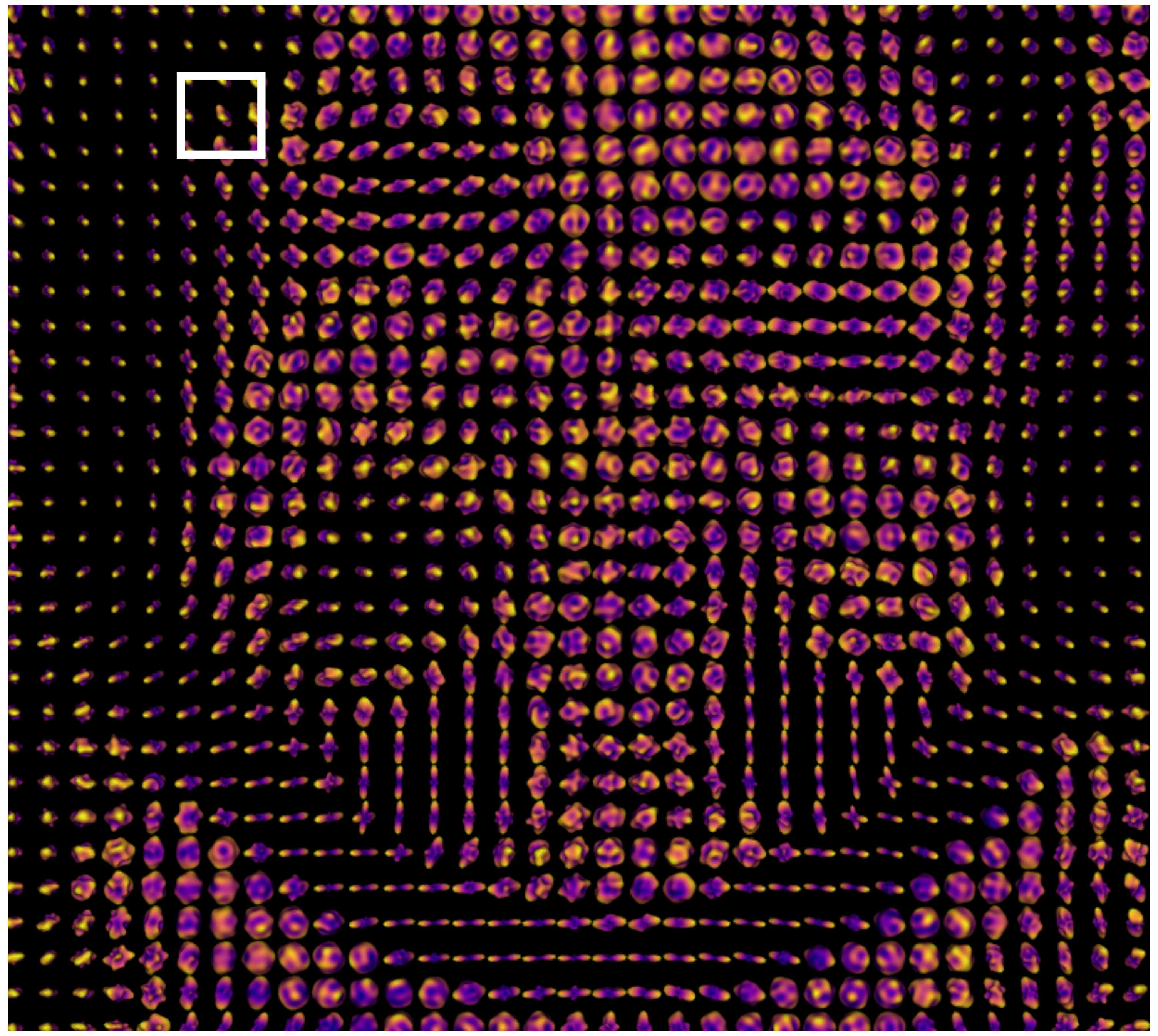
Experiment - Group difference analysis



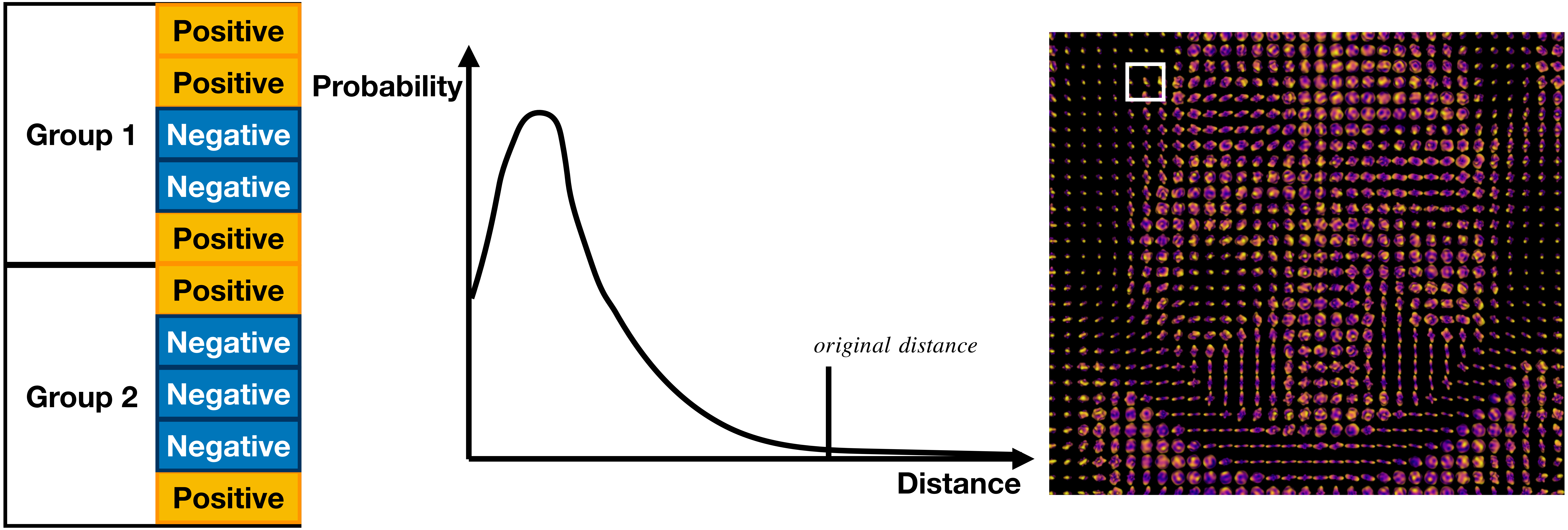


Experiment - Group difference analysis

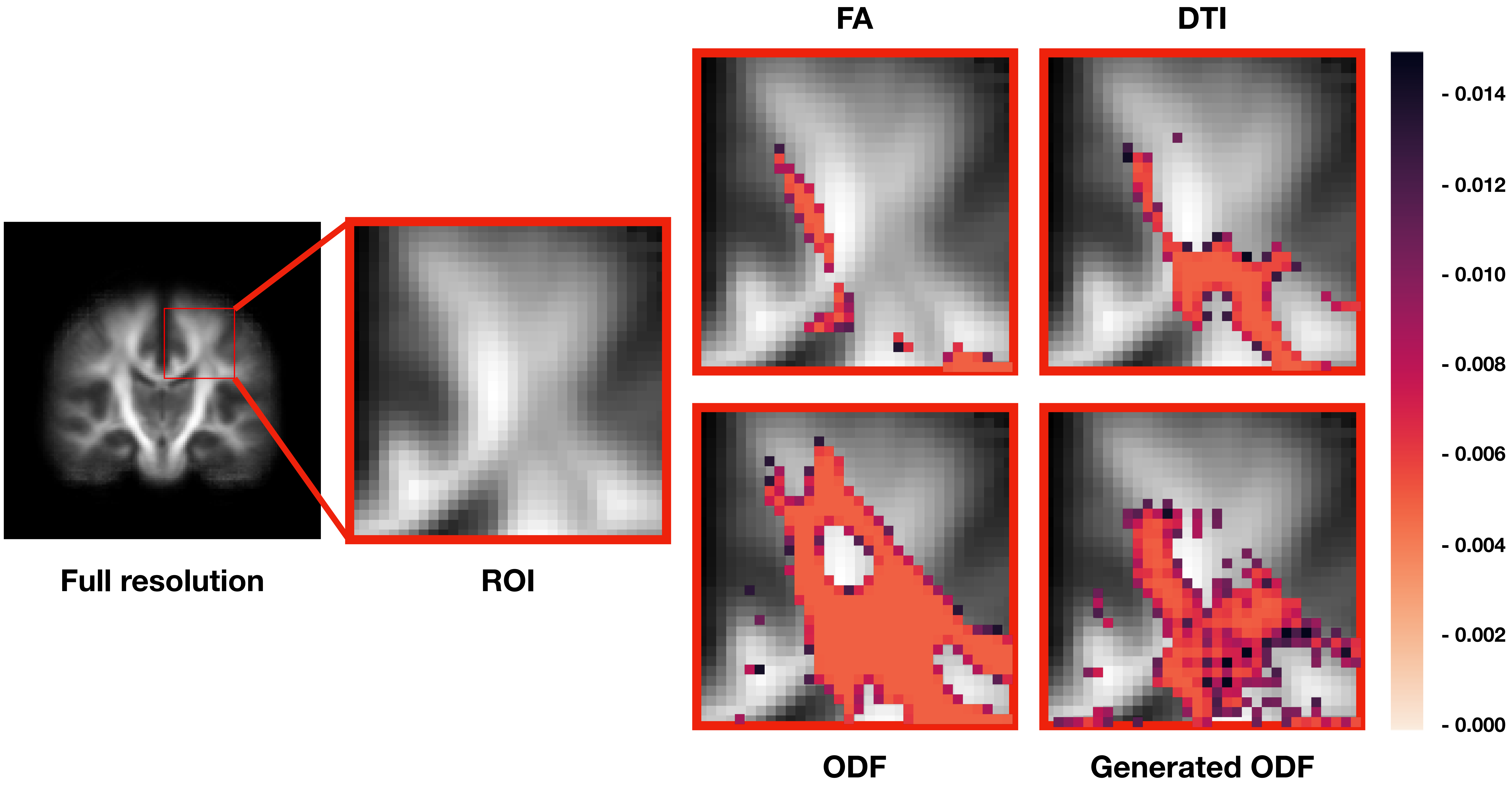




Experiment - Group difference analysis



Experiment - Group difference analysis



Our main contribution