Flow Matching from dumnies

Sometimes you gotta go with the flow...

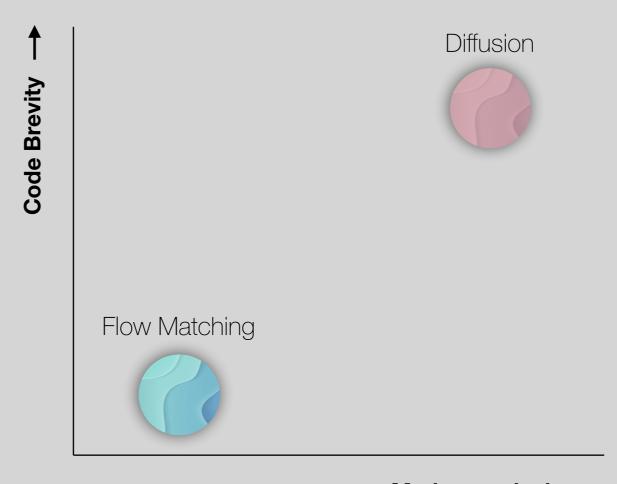




Why do Flow Matching 101...

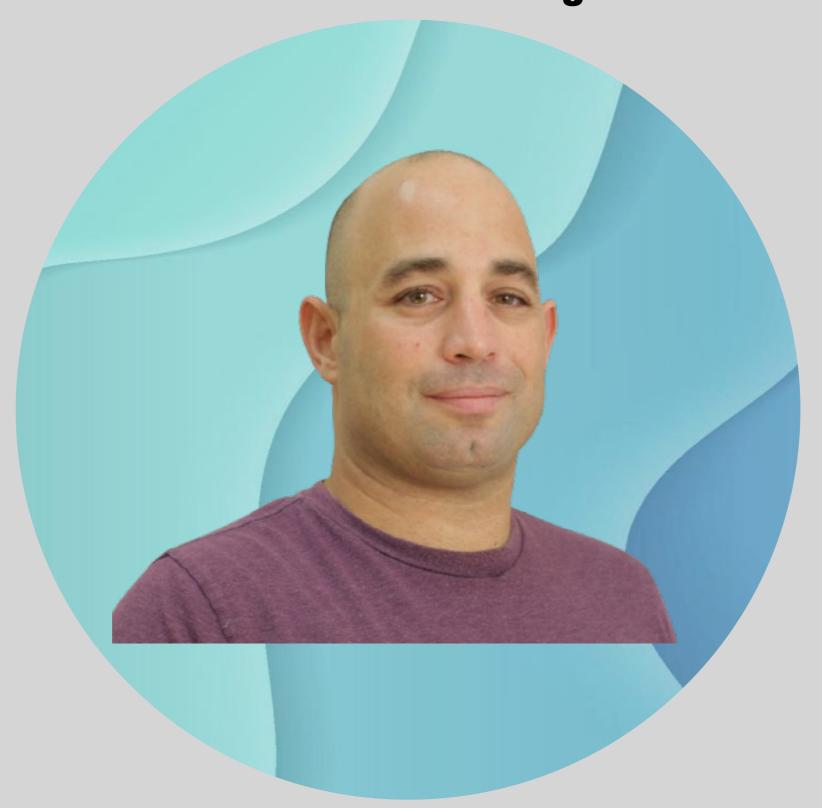


Why do Flow Matching 102...



Math complexity →

Join the Flow Matching Cult



Source: Yaron Lipman















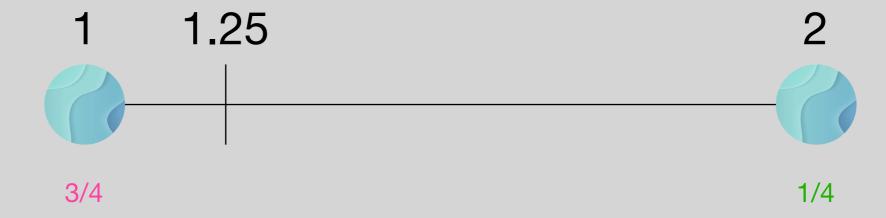


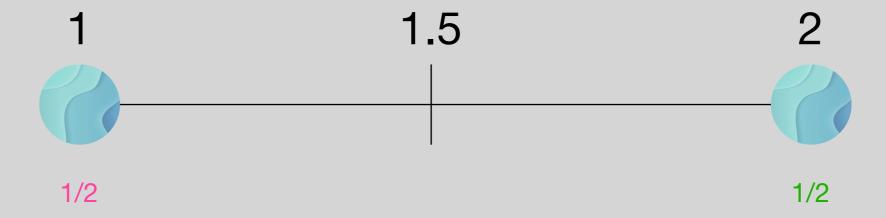


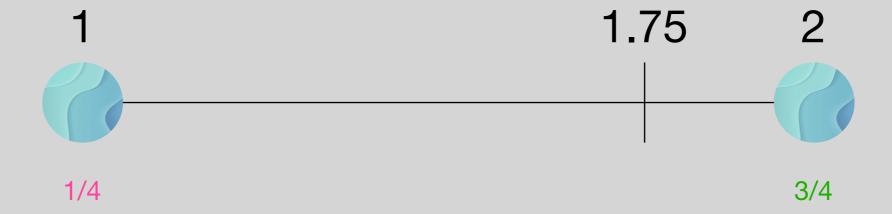
Here are the 3 numbers

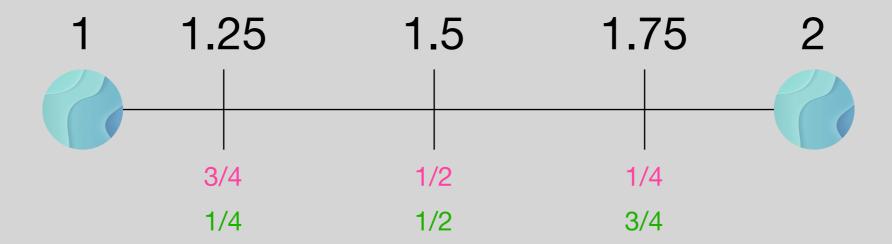


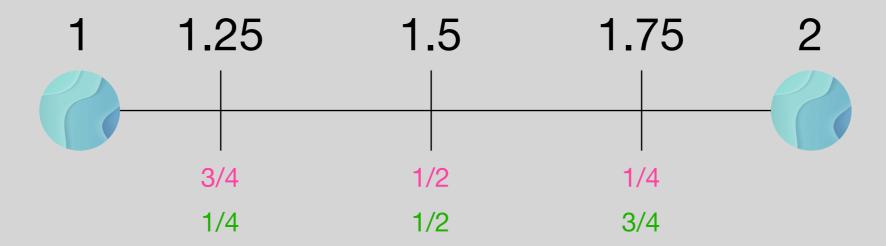
How do you get them?







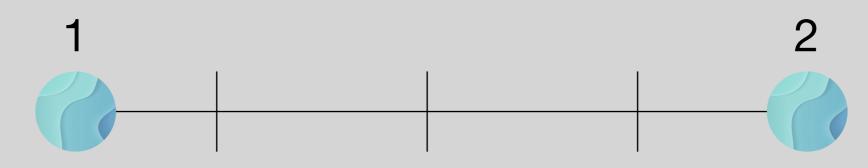




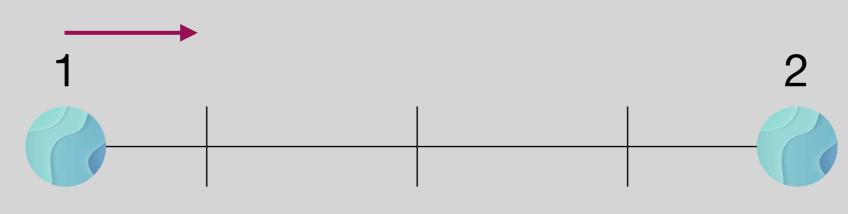
$$\pi_t = t \cdot \pi_1 + (1 - t) \cdot \pi_0$$



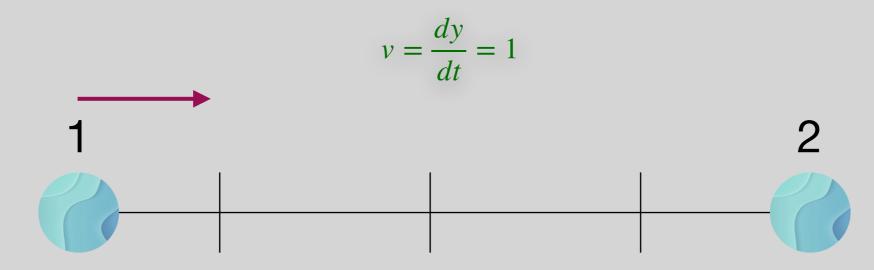
One more way!



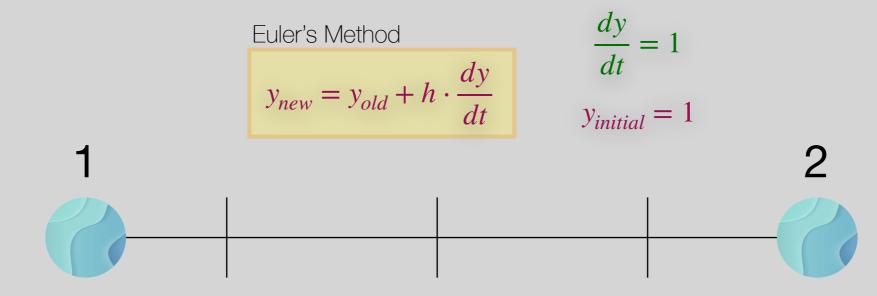
One more way!



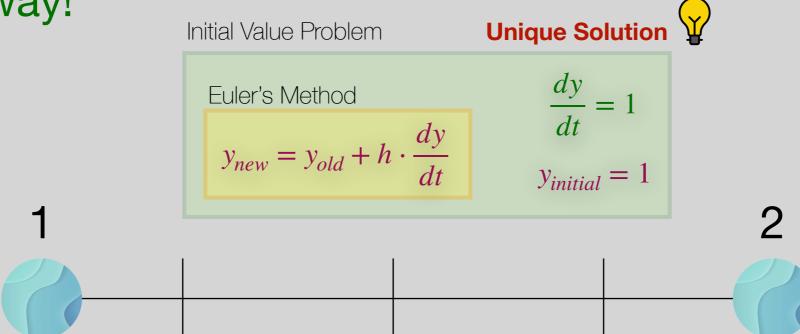
One more way!



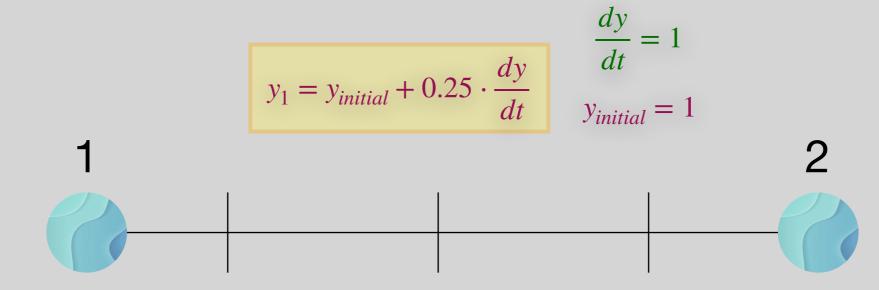
One more way!



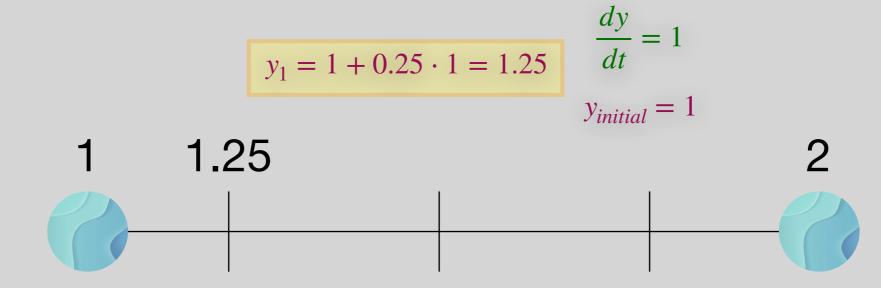
One more way!



One more way!



One more way!



One more way!

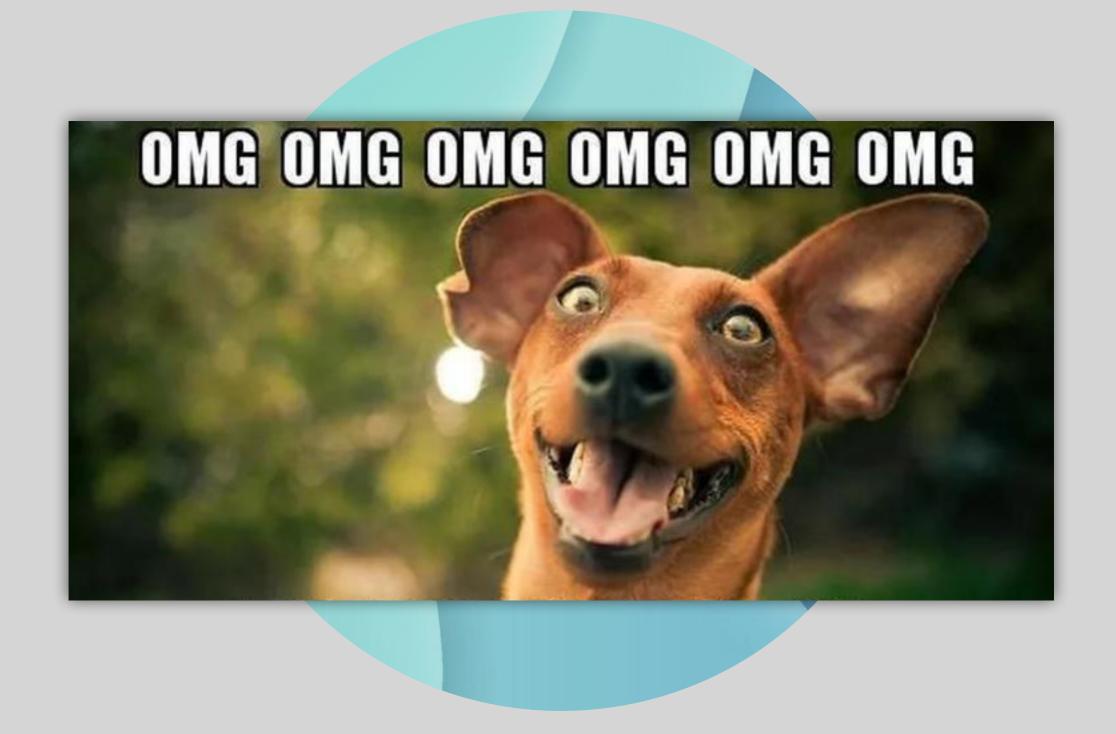
$$y_2 = 1.25 + 0.25 \cdot 1 = 1.5$$

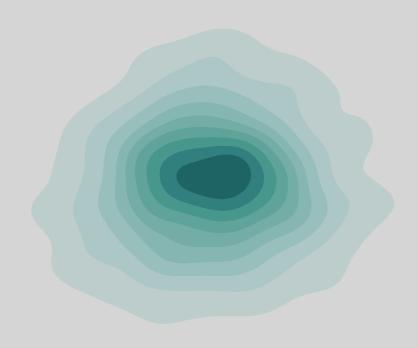


One more way!

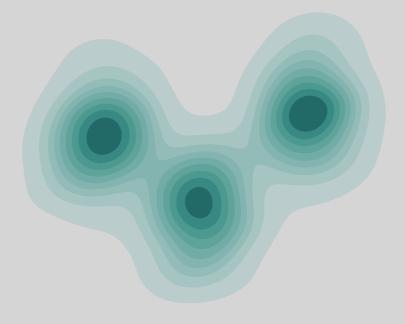
$$y_3 = 1.5 + 0.25 \cdot 1 = 1.75$$



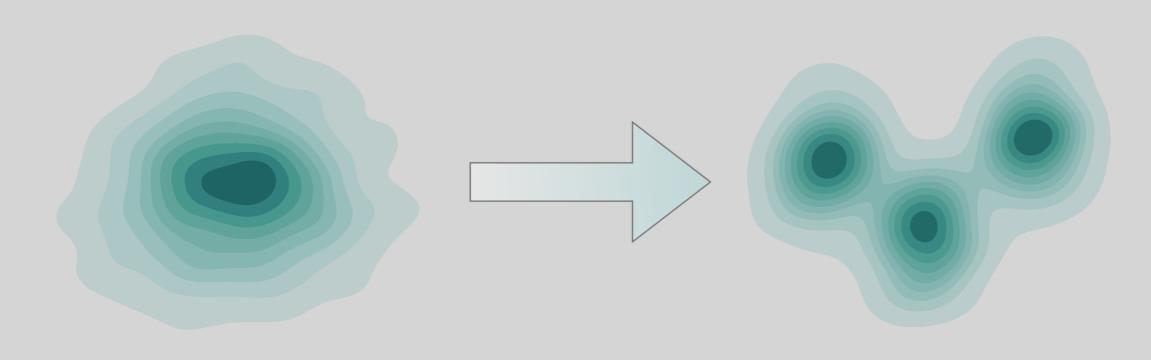




Source Distribution π_0



Target Distribution π_1

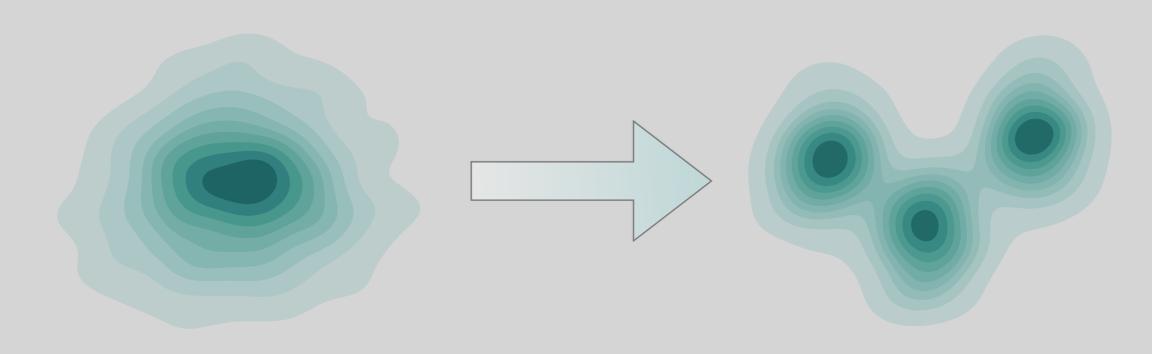


Source Distribution

 π_0

Target Distribution

 π_1



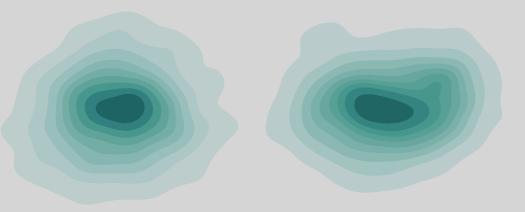
Source Distribution

 π_0

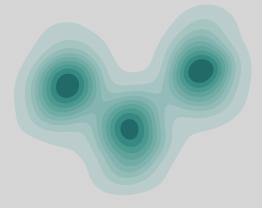
Target Distribution

 π_1

$$\pi_t = t \cdot \pi_1 + (1 - t) \cdot \pi_0$$

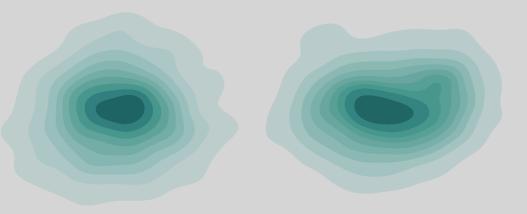


Source Distribution

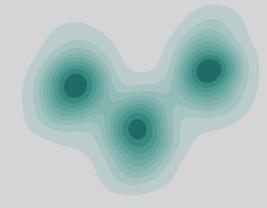


Target Distribution

$$\pi_t = \frac{1}{4} \cdot \pi_1 + \frac{3}{4} \cdot \pi_0$$



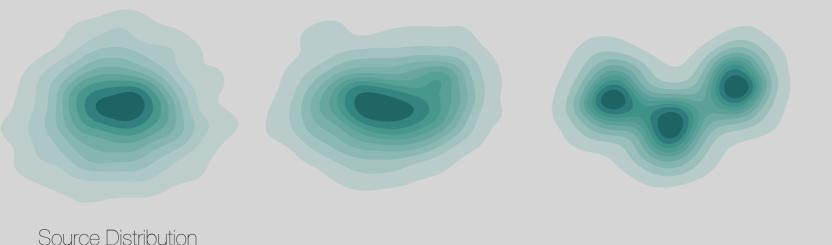
Source Distribution

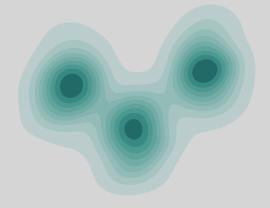


Target Distribution

$$\pi_{\frac{1}{4}} = \frac{1}{4} \cdot \pi_1 + \frac{3}{4} \cdot \pi_0$$

$$\pi_{\frac{1}{4}} = \pi_0 + \frac{1}{4} \cdot \nabla \pi_t$$

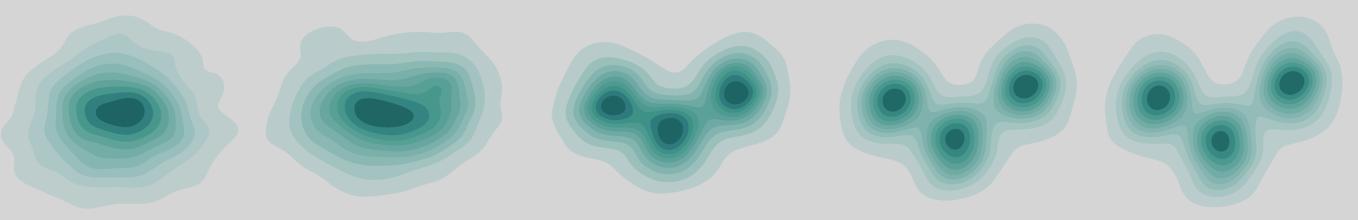




Target Distribution

$$\pi_{\frac{1}{4}} = \frac{1}{2} \cdot \pi_1 + \frac{1}{2} \cdot \pi_0$$

$$\pi_{\frac{1}{2}} = \pi_{\frac{1}{4}} + \frac{1}{4} \cdot \nabla \pi_t$$

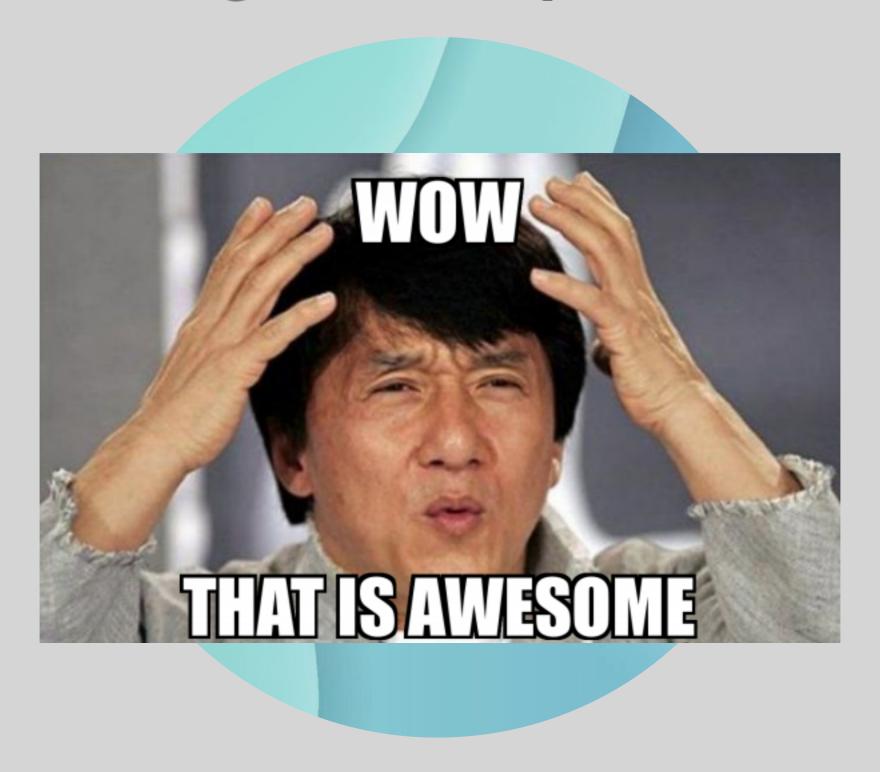


Source Distribution Target Distribution

$$\pi_{\frac{3}{4}} = \frac{3}{4} \cdot \pi_1 + \frac{1}{4} \cdot \pi_0$$

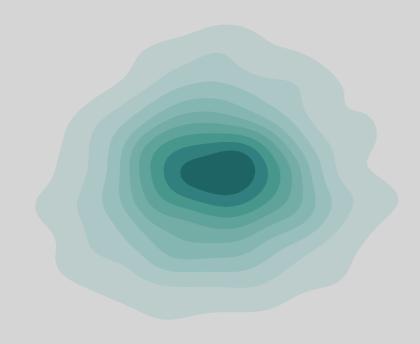
$$\pi_{\frac{3}{4}} = \pi_{\frac{1}{2}} + \frac{1}{4} \cdot \nabla \pi_t$$

Flow Matching is So Simple!

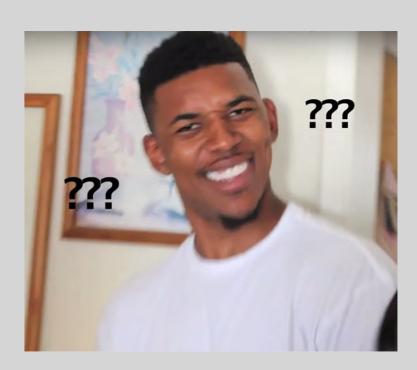


Source: makeameme.org

However...

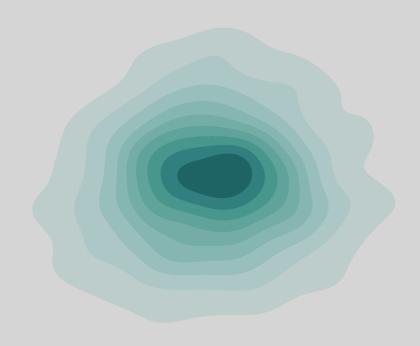


Source Distribution

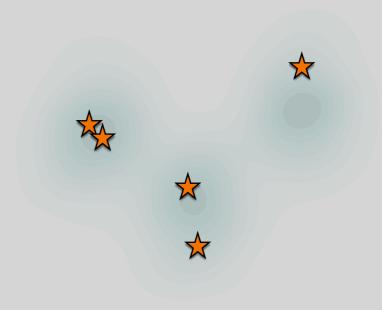


Target Distribution???

However...

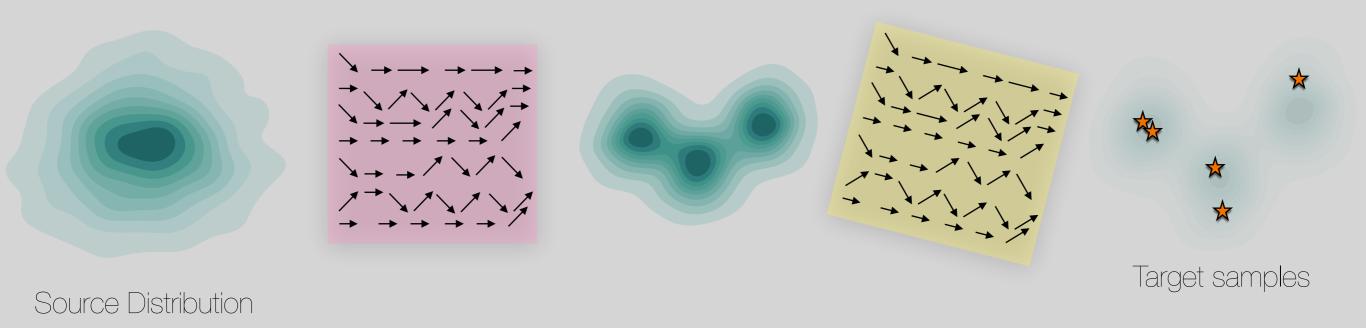


Source Distribution

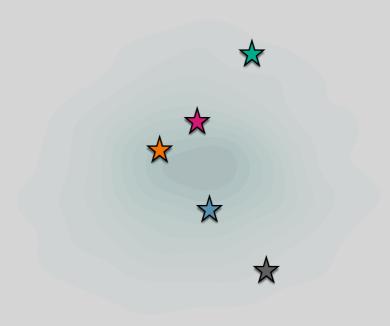


Target samples

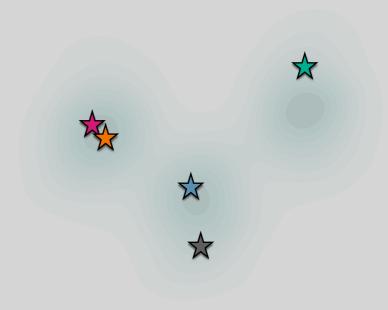
Can we get the velocity to get to intermediates?



Solution 101: Random coupling

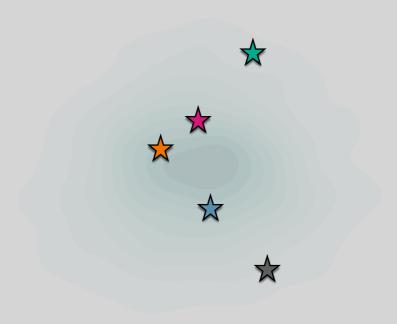


Source Samples

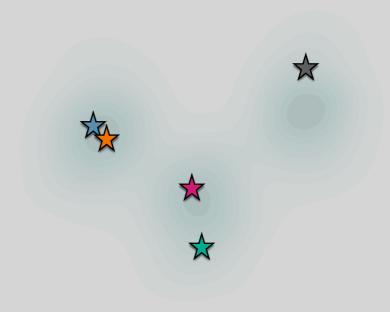


Target samples

Solution 101: Random coupling



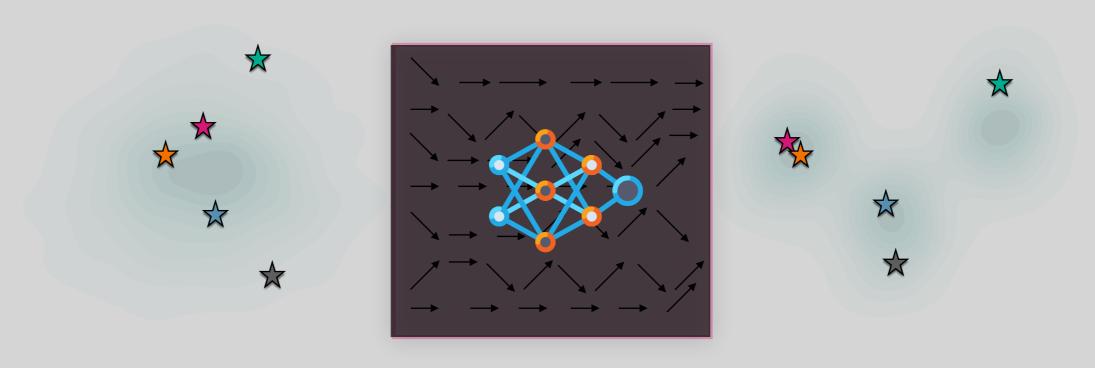




Target samples

Solution 101: Intermediate gradient/ velocity

What are the velocities to make the intermediates?

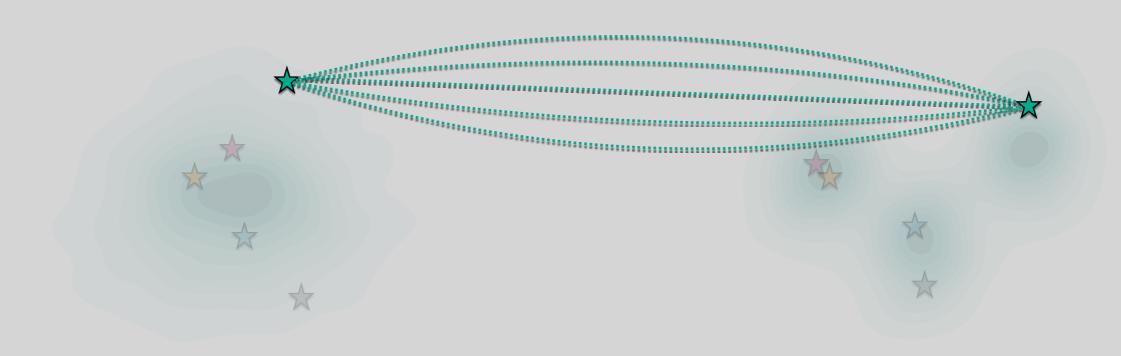


Source Samples

Target samples

!!! Velocity depends on Interpolation paths

Which one to pick?



Source Samples

Target samples

Solution 101: Go linear

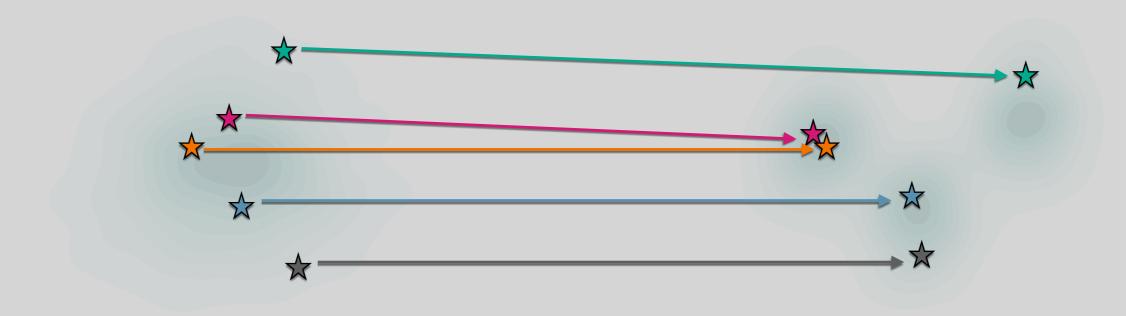


Source Samples

Target samples

Solution 101: Gradients

Model prediction



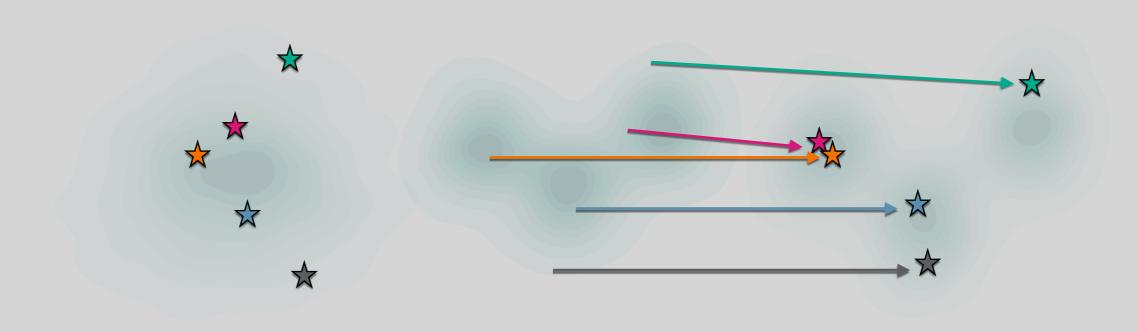
Source Samples

Target samples

 X_{0} $\nabla X_{t} = X_{1} - X_{0}$

Solution 101: Gradients

Model prediction



Source Samples

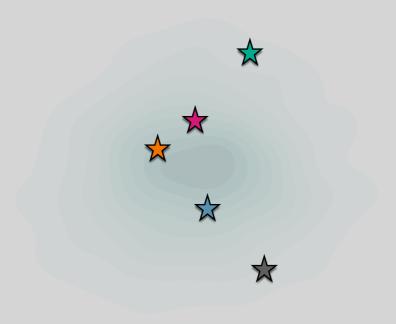
 X_0

Target samples

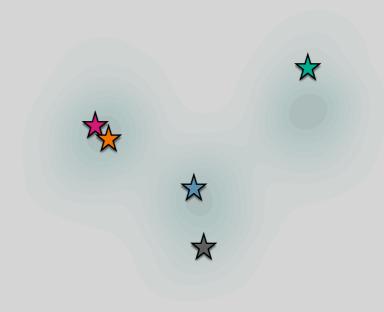
 X_1

 $\nabla X_t = X_1 - X_0$

(1) Random Coupling

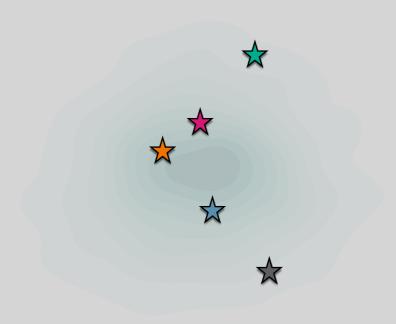


Source Samples X_0

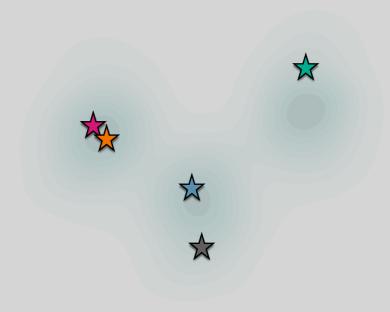


Target samples X_1

(2) Randomly sample t in [0,1)



Source Samples X_0

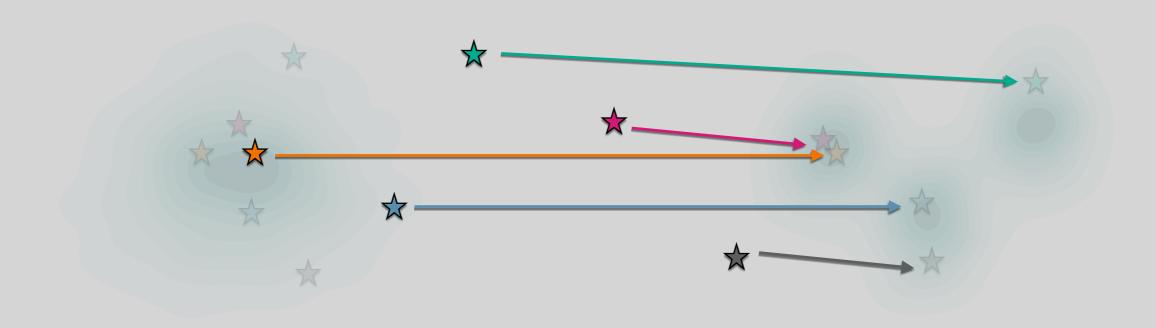


Target samples X_1

(3) Linear interpolation (model input)



(4) Predict Velocity (model output)



Source Samples

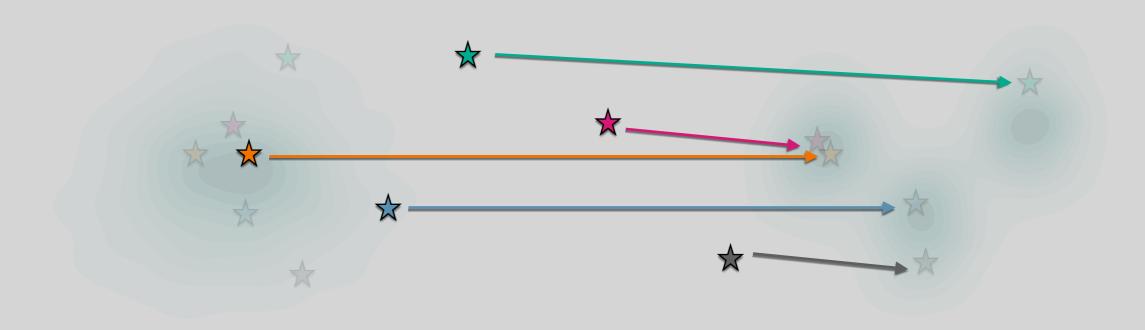
X₀

 $= \nabla X_t$ $u_{\theta}(t)$

Target samples

 X_1

(5) Optimize



Source Samples

 X_0

Target samples

 X_1

$$\mathbb{E}[||u_{\theta}(t) - (X_1 - X_0)||^2]$$

Sampling

Euler's Method

$$x_{next} = x_{old} + \frac{1}{num_steps} \cdot u_{\theta}(t)$$

$$x_{initial} \sim \mathcal{N}(0,I)$$

```
## Setting up the flow matching pipeline ##

class FlowMatchingPipeline:
    """Implements the Flow Matching pipeline"""

def __init__(self):
    """Constructor"""
    self.model = model()
    self.optim = torch.optim.AdamW(self.model.parameters(), lr=1e-4)
    self.loss = nn.MSELoss()
```

```
def interpolate(self, x1, t):
    """Interpolate x1 data from x0 data."""

x0 = torch.randn(*x1.shape, device=x1.device, dtype=x1.dtype)

xt = t * x1 + (1 - t) * x0

vel = x1 - x0

return xt, vel
```

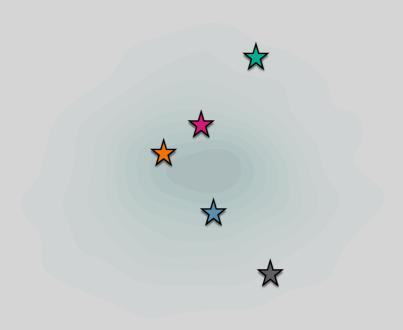
```
def training_step(self, data):
      """Implements one single training step for the model"""
      data = data.to(self.device)
      t = torch.rand(
          data.shape[0],
          dtype=data.dtype,
          device=self.device
10
      ).view(-1,1)
11
      xt, true_vt = self.interpolate(data, t)
12
13
      self.optim.zero_grad()
14
15
      vt = self.model(xt, t)
16
17
      loss = self.loss(true_vt, vt)
18
      loss_val = loss.clone().detach().cpu().item()
19
20
      loss.backward()
21
22
      self.optim.step()
23
24
25
      return loss_val
```

```
@torch.no_grad()
    def sample(self, num_steps, init_val):
      """Samples using euler steps using the model"""
      step_size = 1 / num_steps
 6
      xt = init_val
      for step in range(1, num_steps):
8
        t = torch.tensor(
            [step / num_steps] * init_val.shape[0],
10
            dtype=xt.dtype,
11
            device=self.device
12
        ).view(-1,1)
13
        vt = self.model(xt, t)
14
        xt = xt + step_size * vt
15
16
17
      return xt
18
```

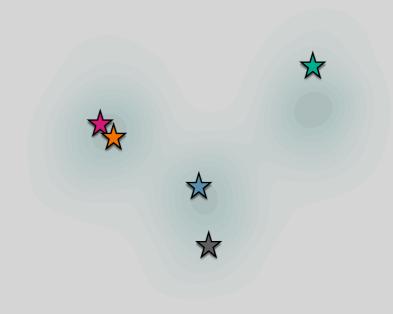
Gimme the Theory...



Recap: Random Coupling

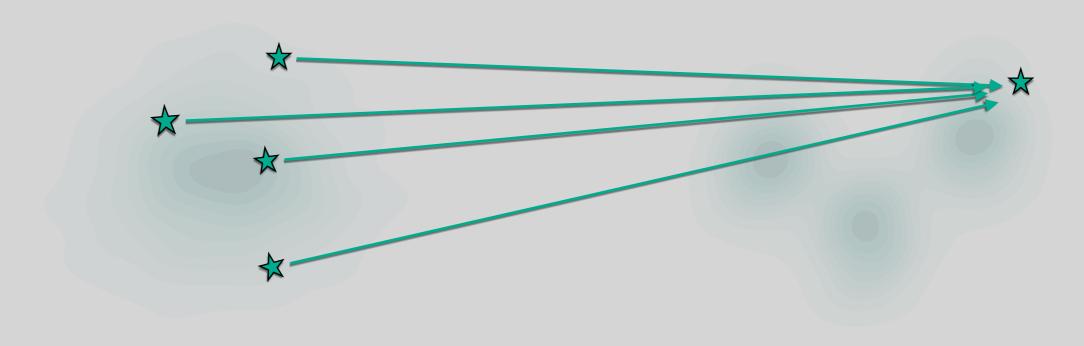






Target samples X_1

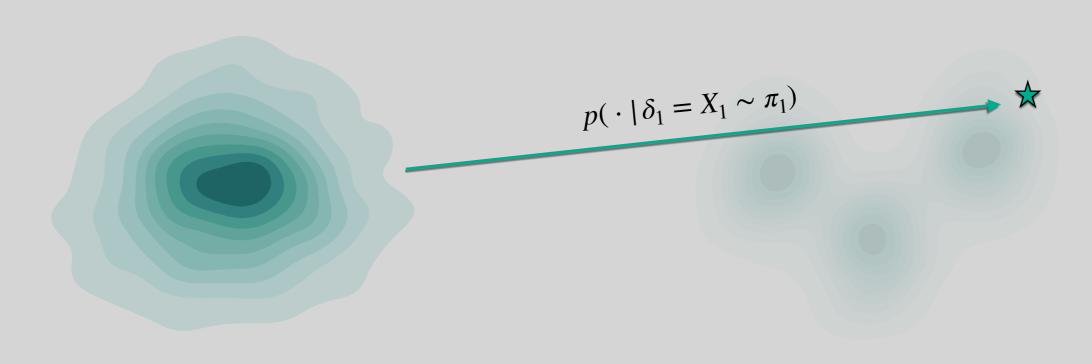
Recap: Random Coupling



Source Samples X_0

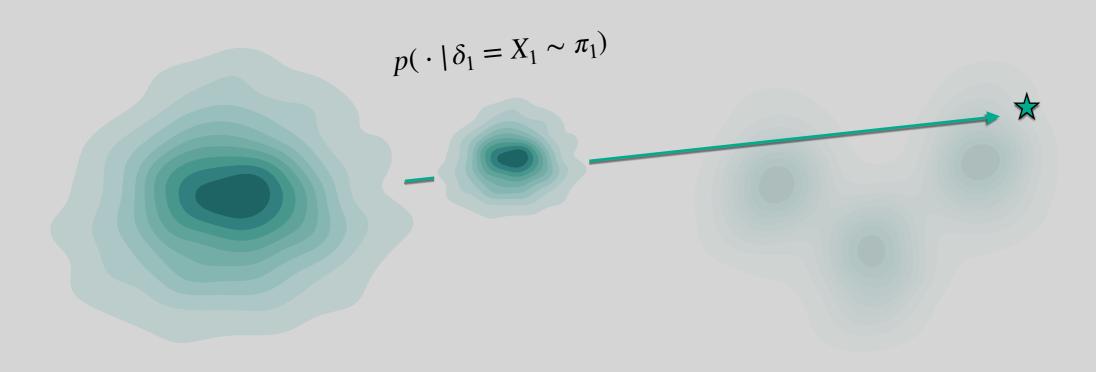
Target samples X_1

Conditional Probability Path



Source Distribution π_0

Conditional Probability Path

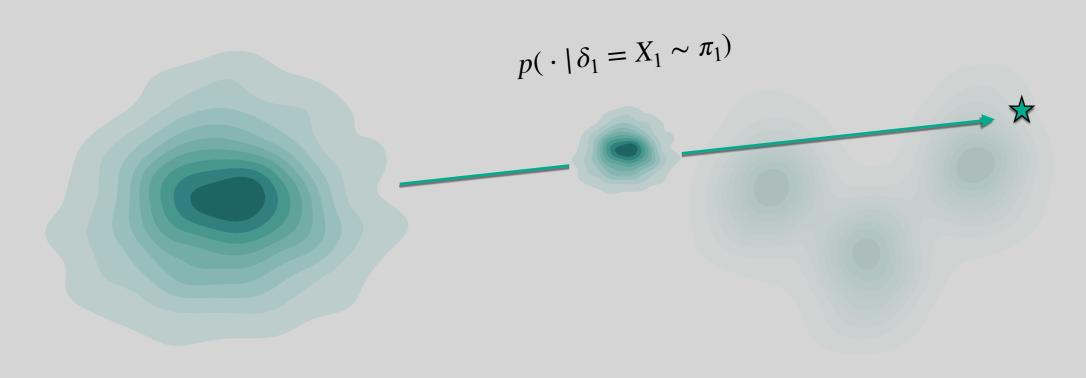


Source Distribution

 π_0

$$X_1 = \delta_1$$

Conditional Probability Path

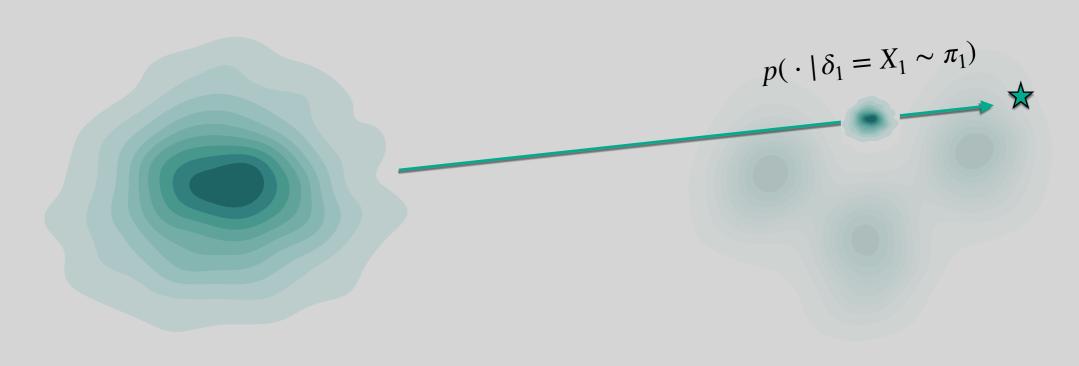


Source Distribution

 π_0

$$X_1 = \delta_1$$

Conditional Probability Path

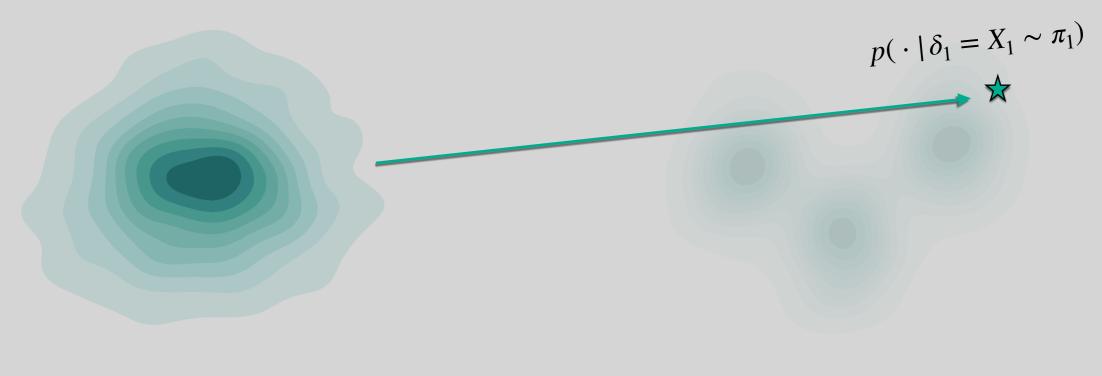


Source Distribution

 π_0

$$X_1 = \delta_1$$

Conditional Probability Path

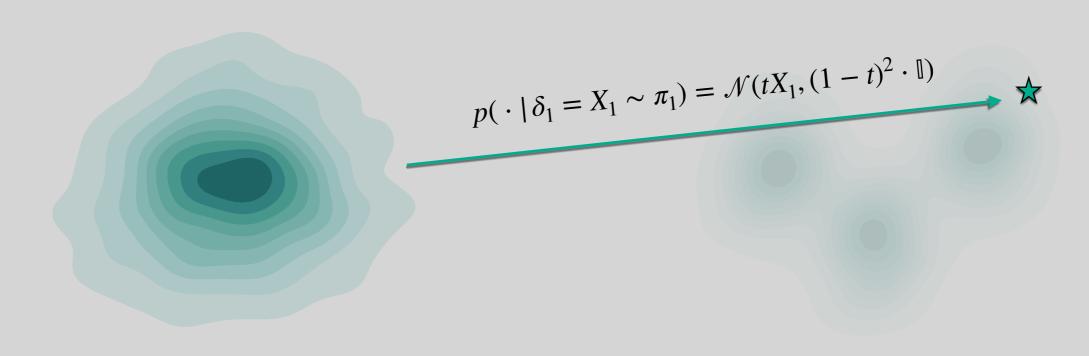


Source Distribution

 π_0

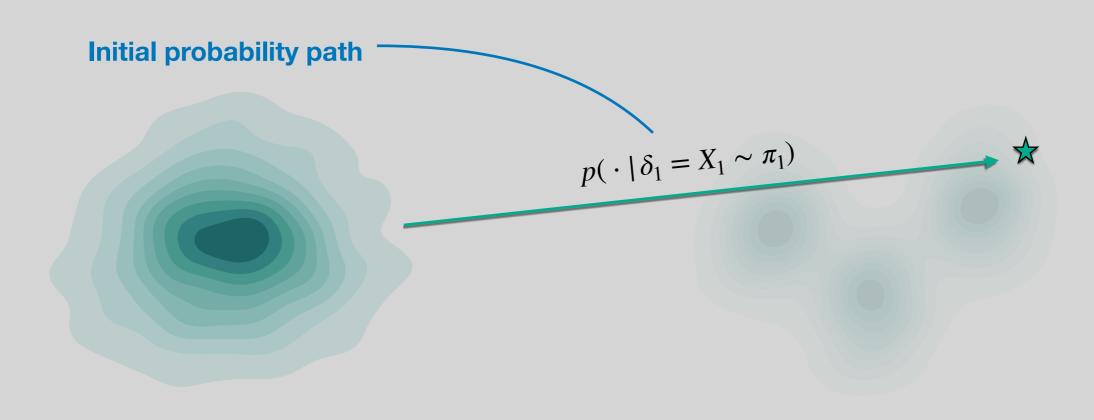
$$X_1 = \delta_1$$

Conditional Probability Path



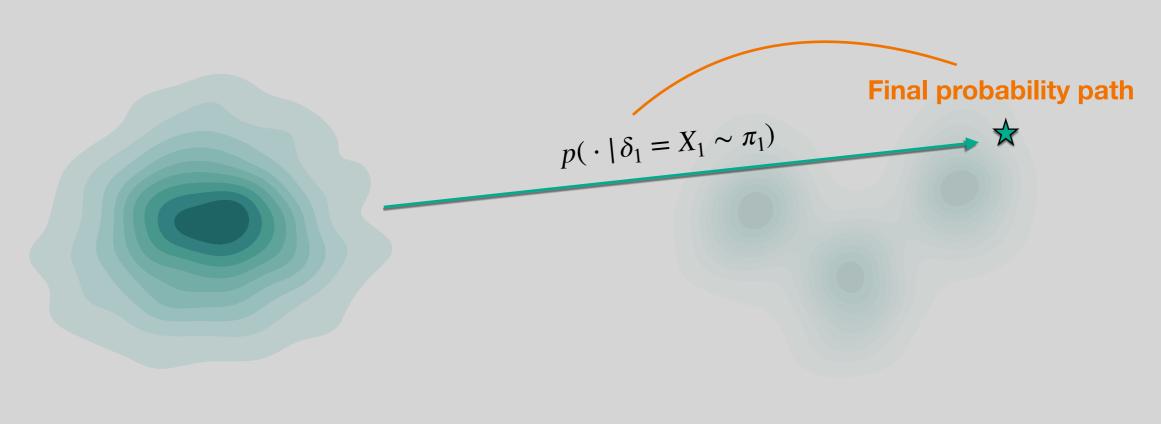
Source Distribution π_0

Conditional Probability Path



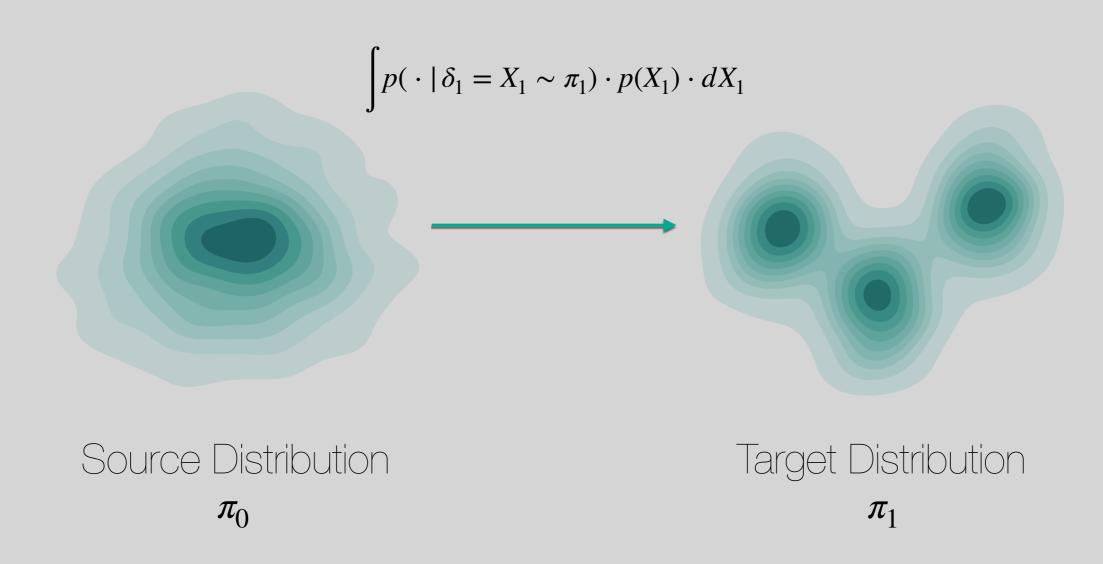
Source Distribution π_0

Conditional Probability Path

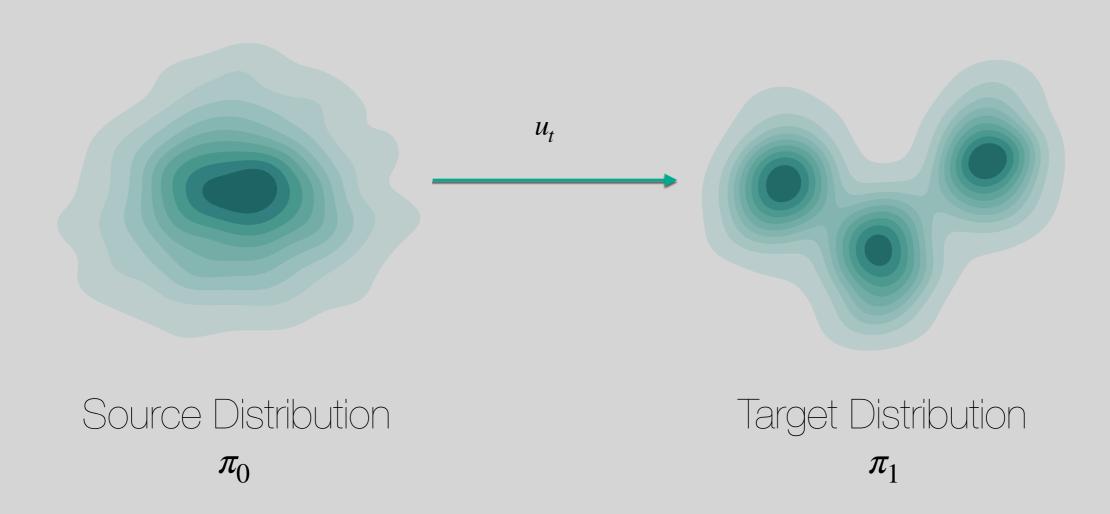


Source Distribution π_0

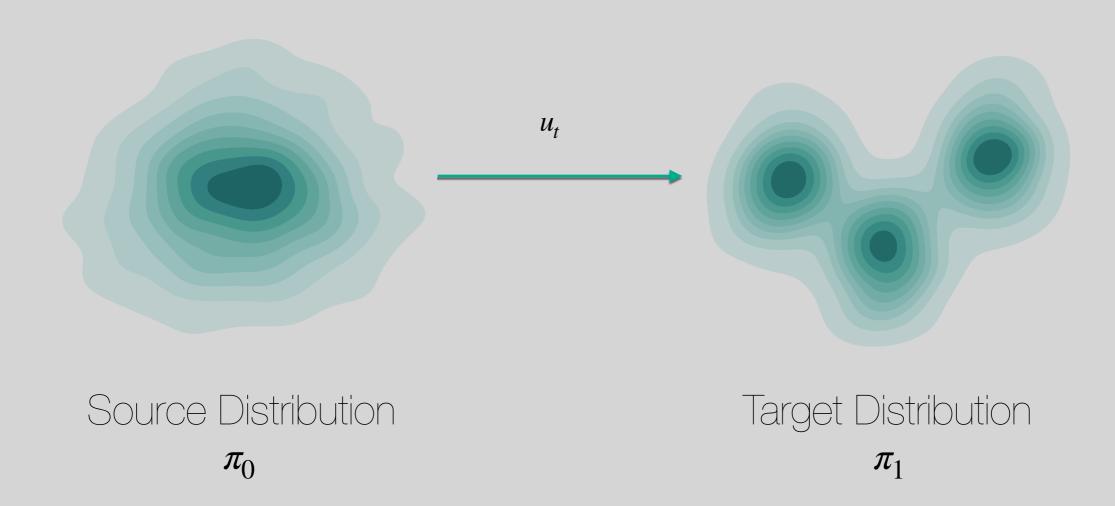
Marginal Probability Path



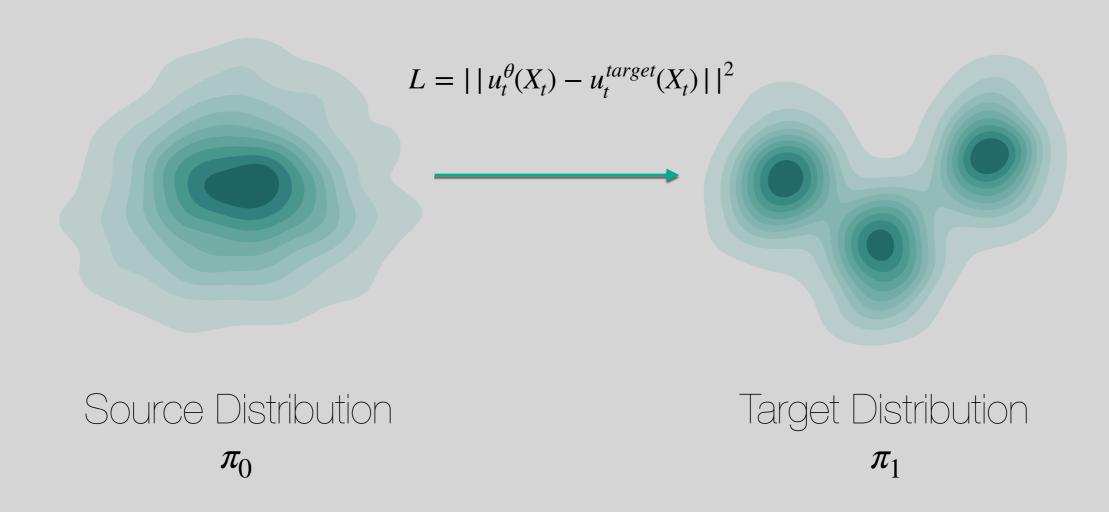
Marginal Velocity Field



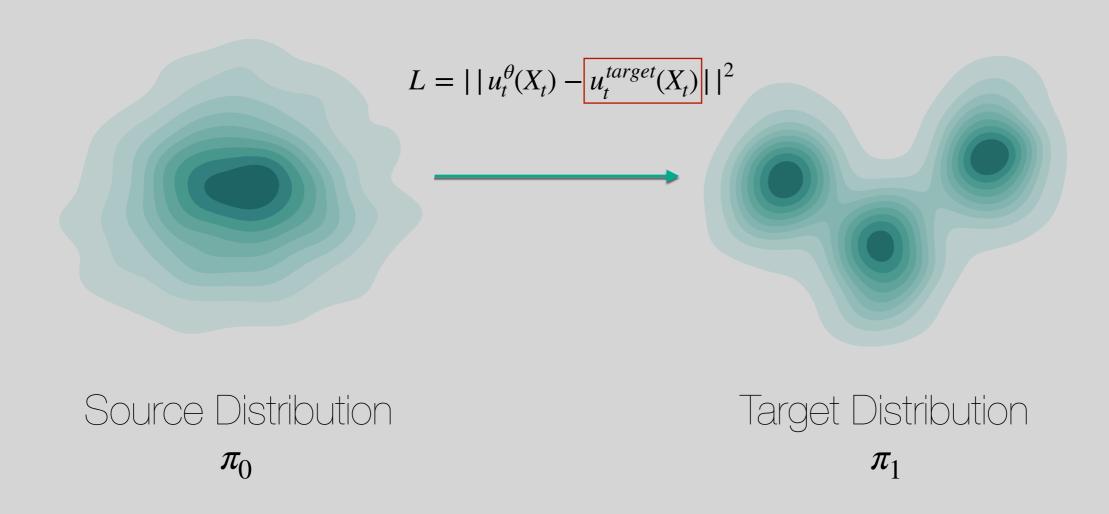
Marginal Velocity Field: Follows marginal probability path



Marginal Velocity Field: Minimize

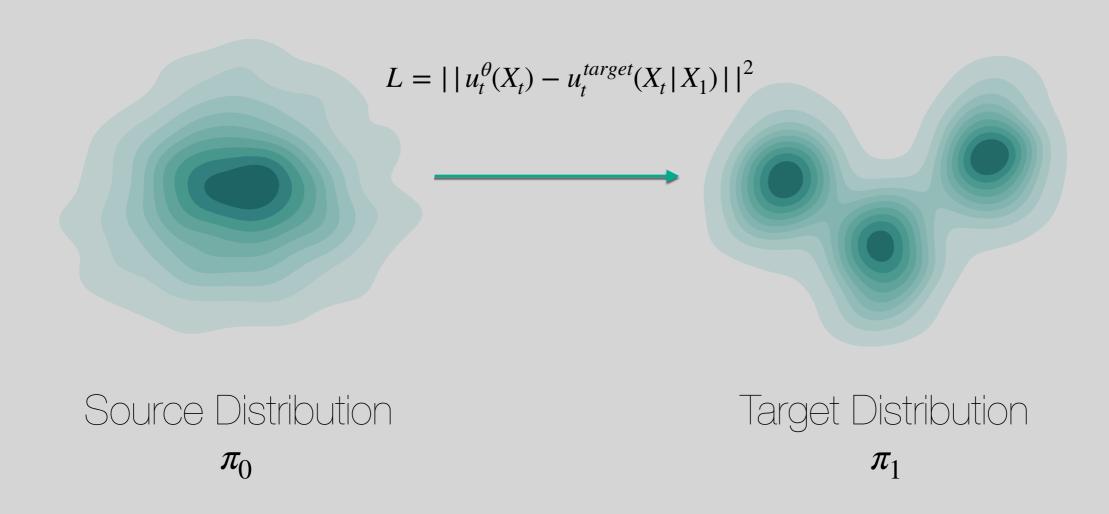


Marginal Velocity Field



Theory of Flow Matching 101...

Conditional Velocity Field

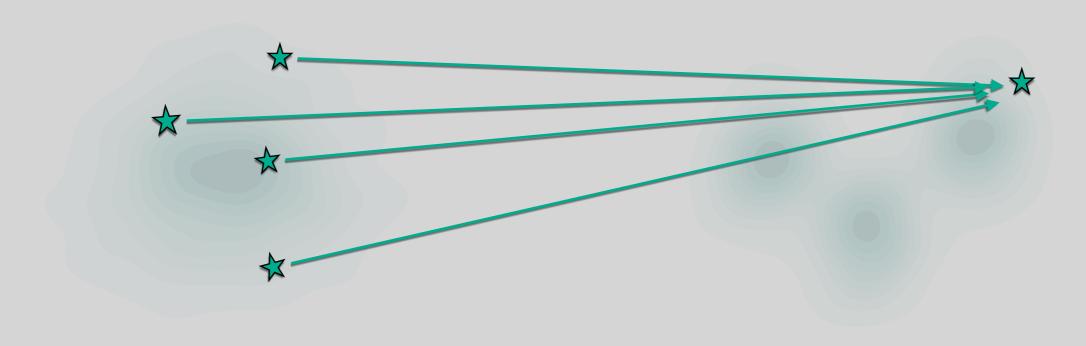


Theory of Flow Matching 101...

Conditional Velocity Field for optimal transport path



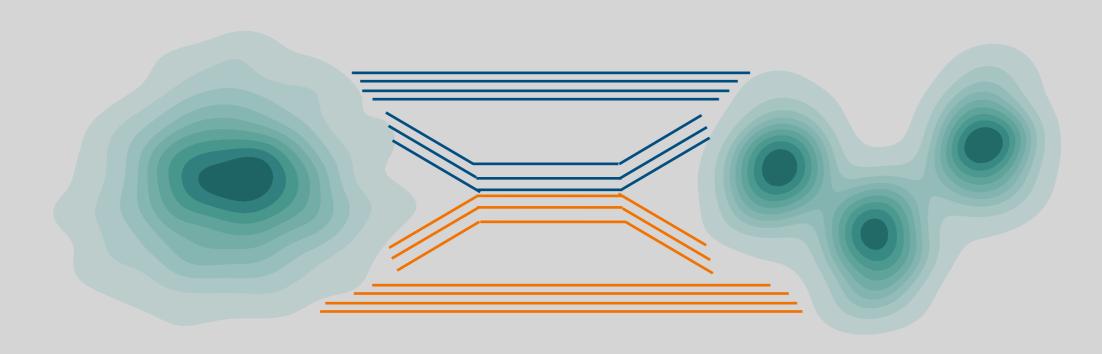
Recap: Random Coupling



Source Samples X_0

Target samples X_1

Learnt Vector Fields

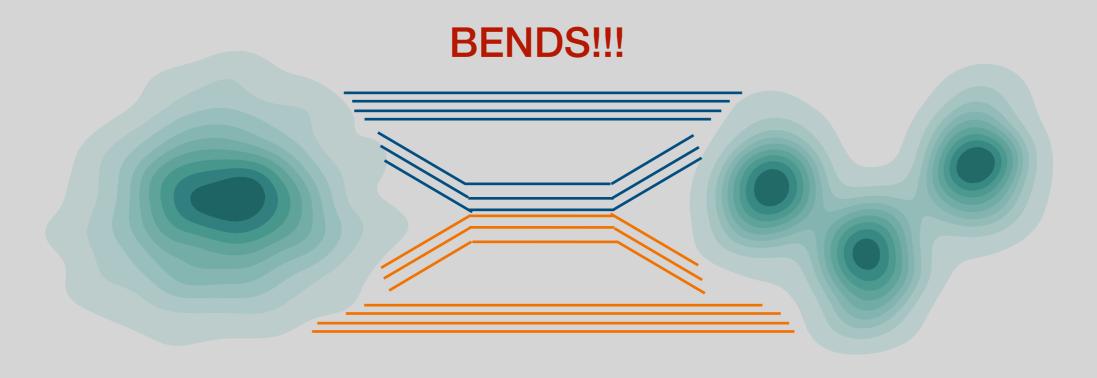


Source Distribution

 π_0

Target distribution

Learnt Vector Fields



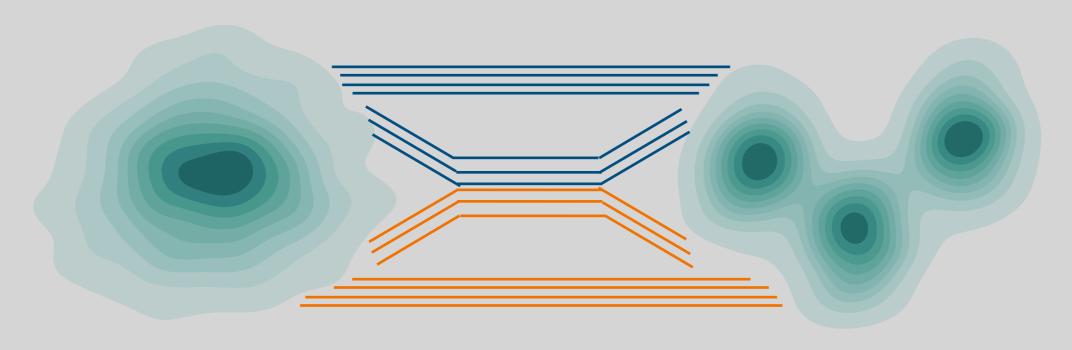
Source Distribution

 π_0

Target distribution

Learnt Vector Fields

Requires more Sampling steps



Source Distribution

 π_0

Target distribution

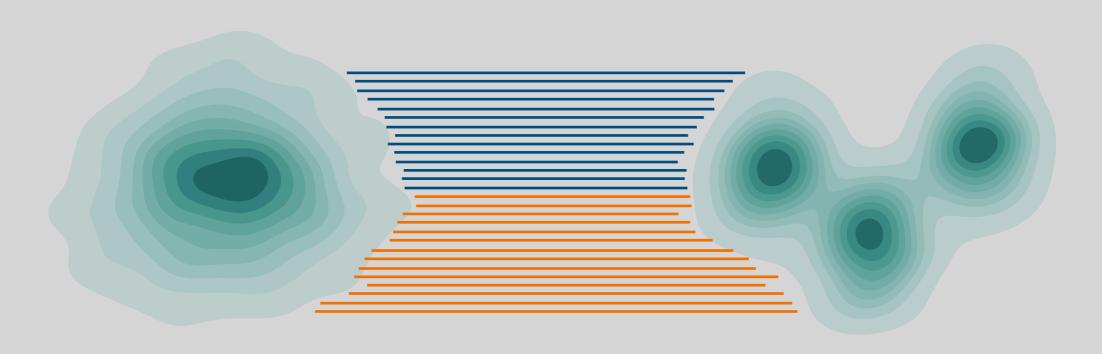
Distill with straight pairs



Source Samples X_0

Target samples X_1

Learnt Vector Fields

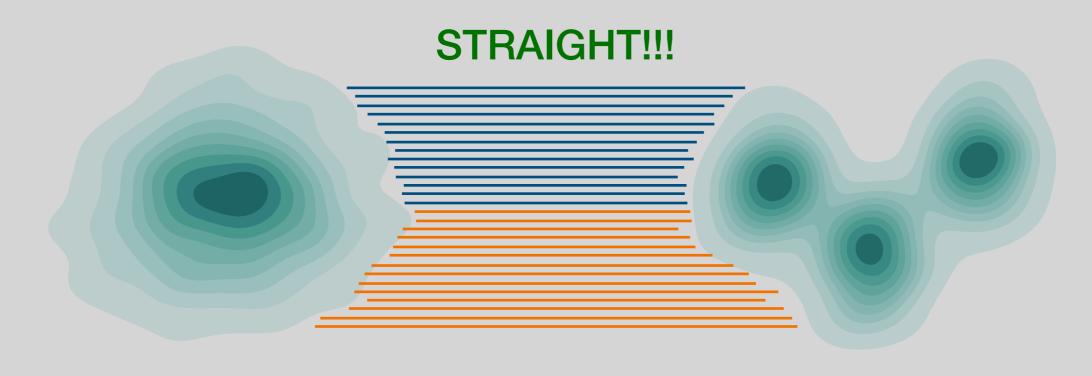


Source Distribution

 π_0

Target distribution

Learnt Vector Fields

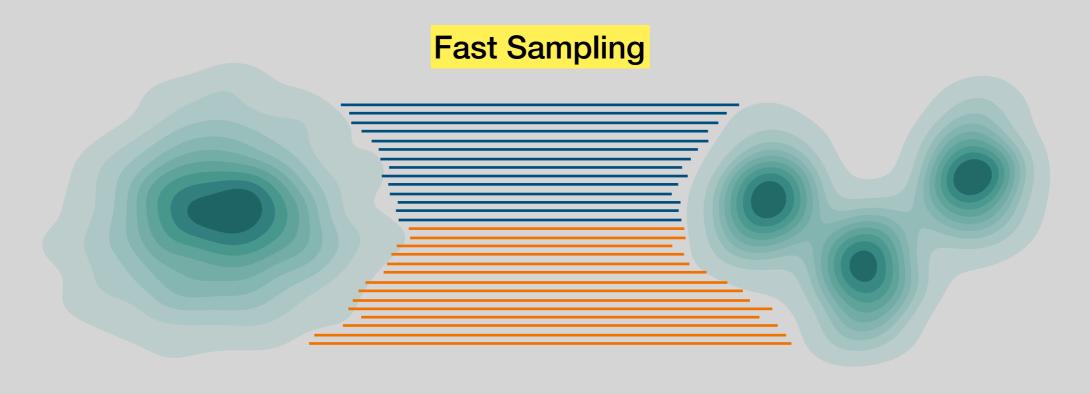


Source Distribution

 π_0

Target distribution

Learnt Vector Fields



Source Distribution

 π_0

Target distribution

Update 102: Better ODE Solvers

Recap: Sampling

Euler's Method

$$x_{next} = x_{old} + \frac{1}{num_steps} \cdot u_{\theta}(t)$$

$$x_{initial} \sim \mathcal{N}(0,I)$$

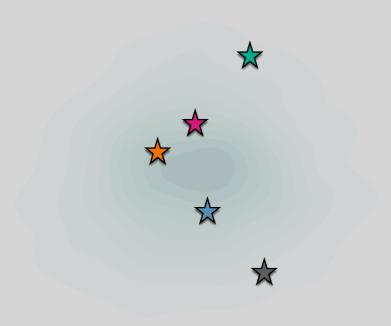
Update 102: Better ODE Solvers

Why not use better ones?

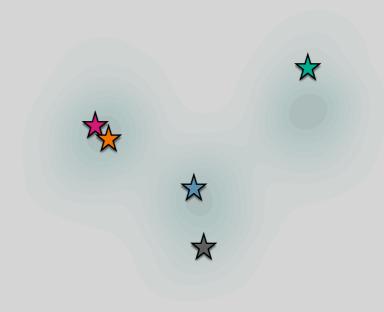
Heun Method

RK Method

Recap: Randomly sample t in [0,1)

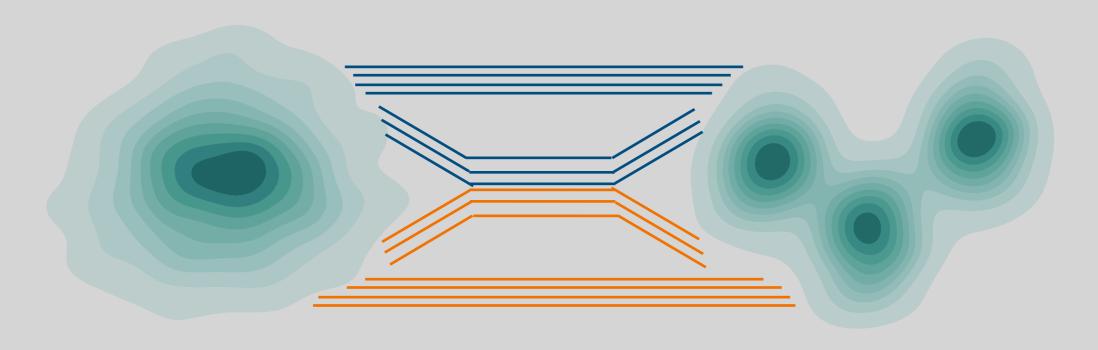






Target samples X_1

Recap: Learnt Vector Fields

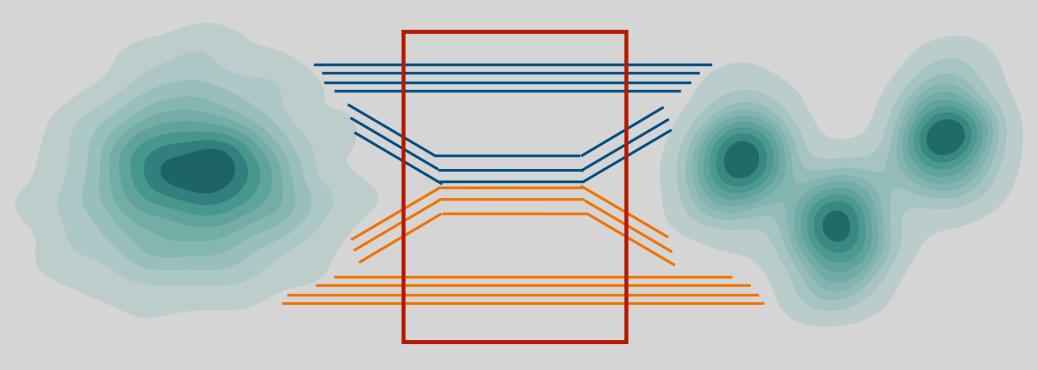


Source Distribution

 π_0

Target distribution

Change in single path mostly in the middle



Source Distribution

 π_0

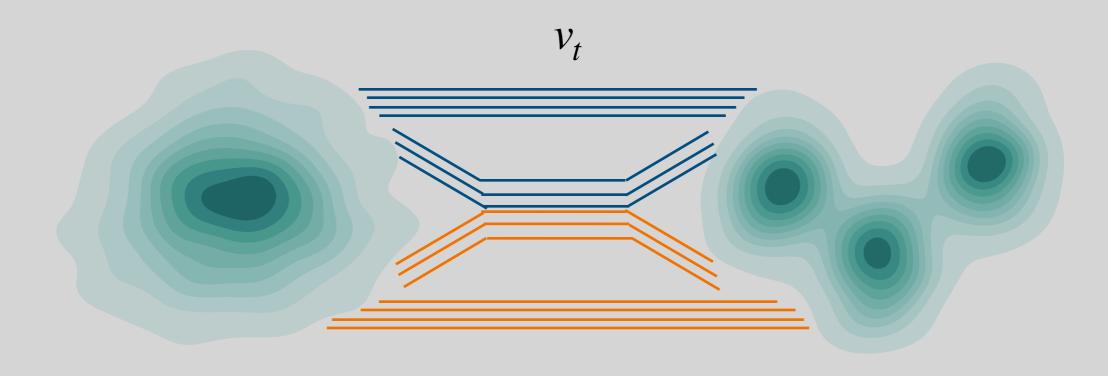
Target distribution

Logit-Normal Sampling

$$t = \frac{1}{1 + \exp(u)}$$

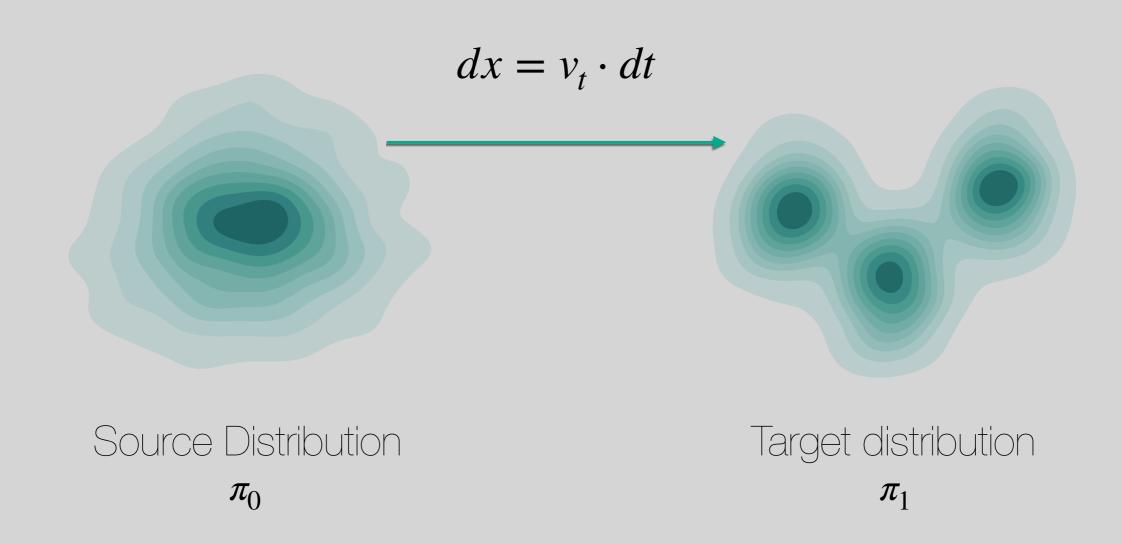
$$u \sim \mathcal{N}(0,1)$$

Flow Matching: Learn a vector field



Source Distribution π_0

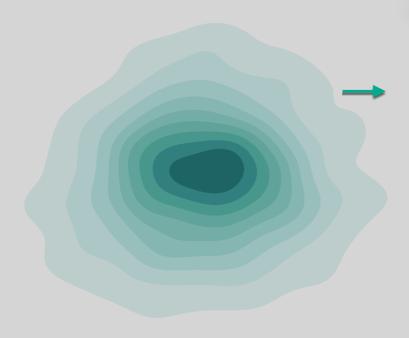
Flow Matching Sampling: Solving an ODE



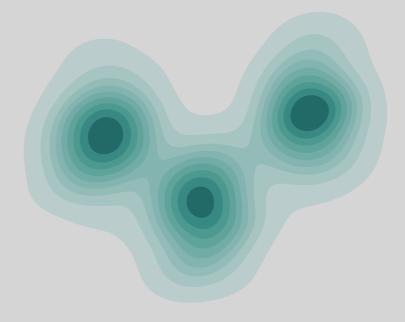
Flow Matching Sampling: Solving an ODE

$$dx = v_t \cdot dt$$

$$x_{t+h} = x_t + h \cdot v_t$$



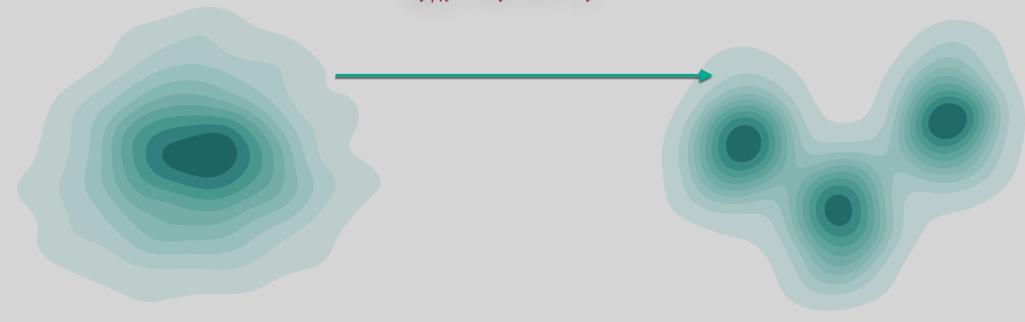
Source Distribution π_0



Flow Matching Sampling: Solving an ODE

$$dx = v_t \cdot dt$$

$$x_{t+h} = x_t + h \cdot v_t$$



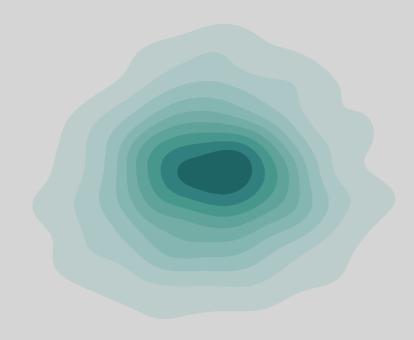
Source Distribution

 π_0

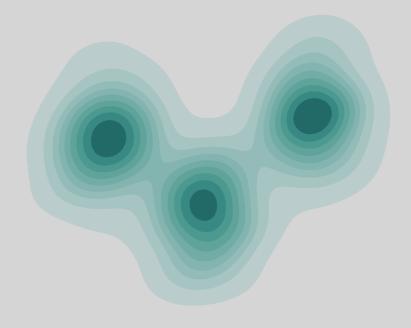
Target distribution

SDE and Diffusion

$$dx = [v_t + \lambda(w_t) \cdot s_t] \cdot dt + w_t \cdot dW$$



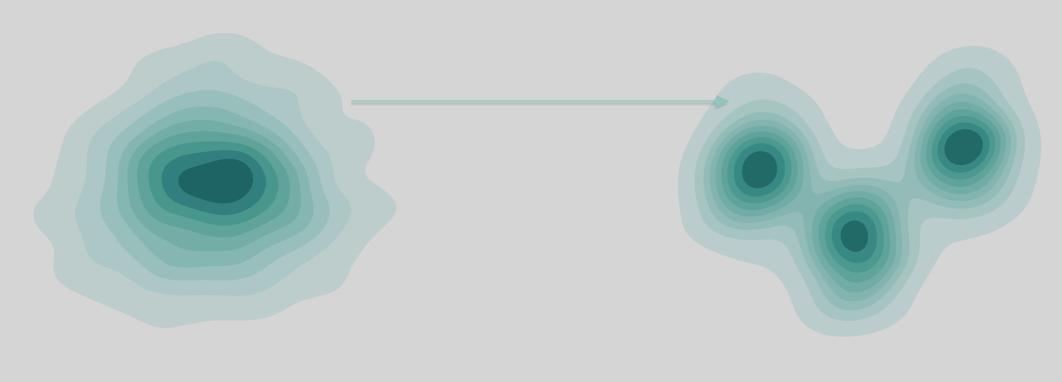
Source Distribution π_0



Target distribution π_1

SDE and Diffusion

$$dx = [v_t + \lambda(w_t) \cdot s_t] \cdot dt + w_t \cdot dW$$



Source Distribution π_0

SDE and Diffusion

$$dx = [v_t + \lambda(w_t) \cdot s_t] \cdot dt + [w_t \cdot dW]$$
Noise

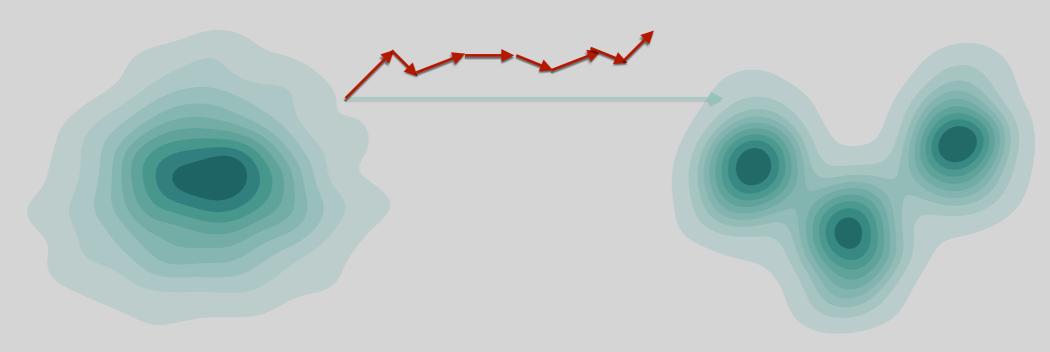


Source Distribution π_0

SDE and Diffusion

$$dx = [v_t + \lambda(w_t) \cdot s_t] \cdot dt + w_t \cdot dW$$

Noise



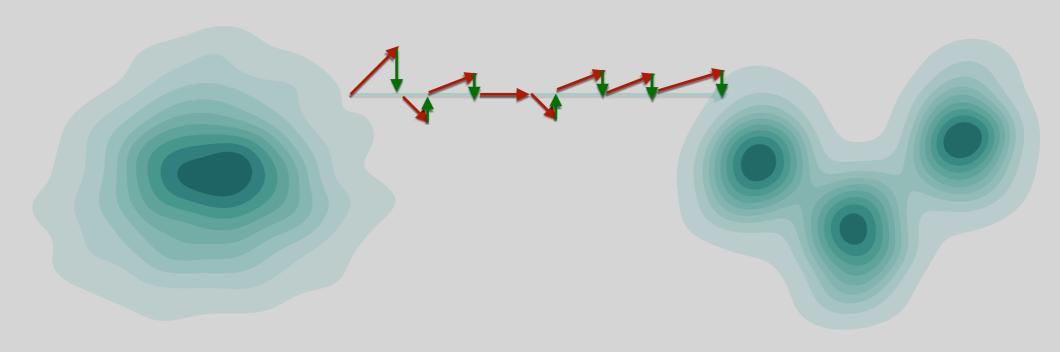
Source Distribution π_0

SDE and Diffusion

Correction

$$dx = [v_t + \lambda(w_t) \cdot s_t] \cdot dt + w_t \cdot dW$$

Noise



Source Distribution π_0

Predict Score
$$dx = [v_t + \lambda(w_t) \cdot \dot{s}_t] \cdot dt + w_t \cdot dW$$

Diffusion Models

Predict Score
$$dx = [v_t + \lambda(w_t) \cdot \dot{s}_t] \cdot dt + w_t \cdot dW$$

Fun Fact: Using Tweedie's formula

$$v_t \leftrightarrow s_t$$

$$x_{t+h} = x_t +$$

$$x_{t+h} = x_t + h \cdot (s_t)$$

$$x_{t+h} = x_t + h \cdot (s_t + \frac{1}{\lambda(w_t)} \cdot v_t)$$

Diffusion Models

DDIM Sampler

$$x_{t+h} = x_t + h \cdot (s_t + \frac{1}{\lambda(w_t)} \cdot v_t)$$

$$x_{t+h} = x_t + h \cdot (s_t + \frac{1}{\lambda(w_t)} \cdot v_t) + w_t \cdot \epsilon$$

Diffusion Models

DDPM Sampler

$$x_{t+h} = x_t + h \cdot (s_t + \frac{1}{\lambda(w_t)} \cdot v_t) + w_t \cdot \epsilon$$

Thank you!

