Learning generative models from observations using expectation maximisation

Rozet++ 2024



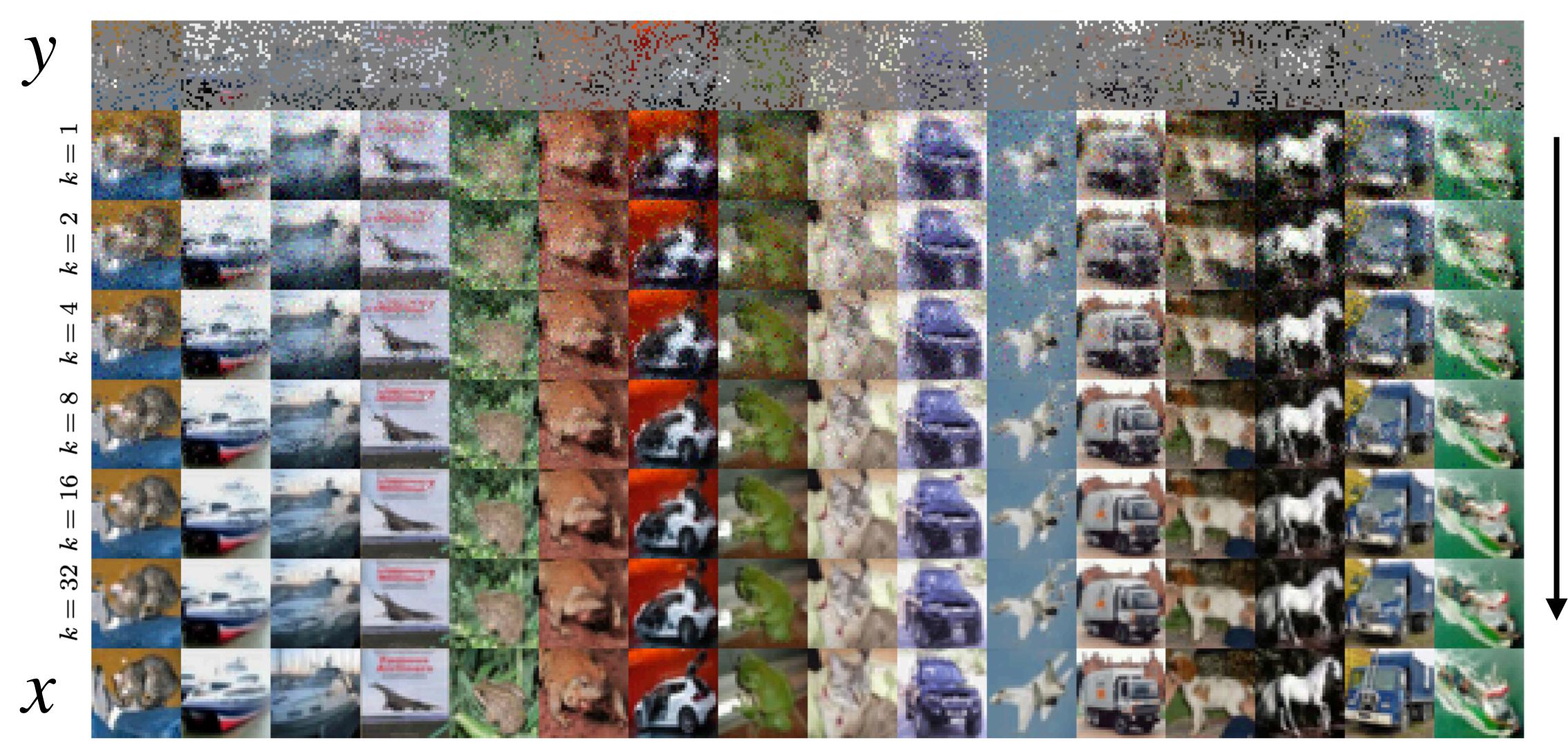
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- Result
- Problem
- Fitting p(x) given only y
- Diffusion
- Algorithm

We only have access to y, a corrupted realisation of a latent x



• It is possible to fit a model for the latents p(x)

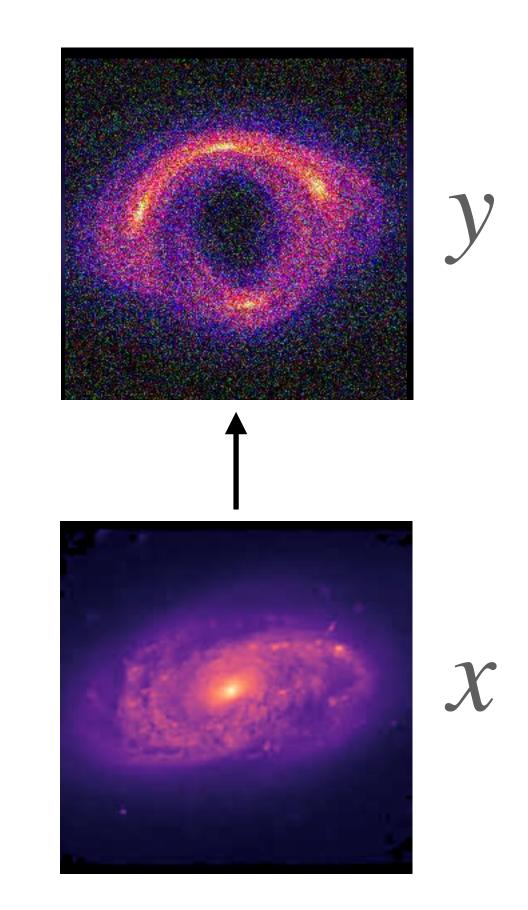
Bayesian inverse problems

• y is a **noisy and corrupted** realisation of x

$$p(x|y) \propto p(y|x) \cdot p(x)$$

• Assumed likelihood of y in terms of x

$$p(y \mid x) = \mathcal{G}[y \mid Ax, \Sigma_y]$$



...which may be different for each x

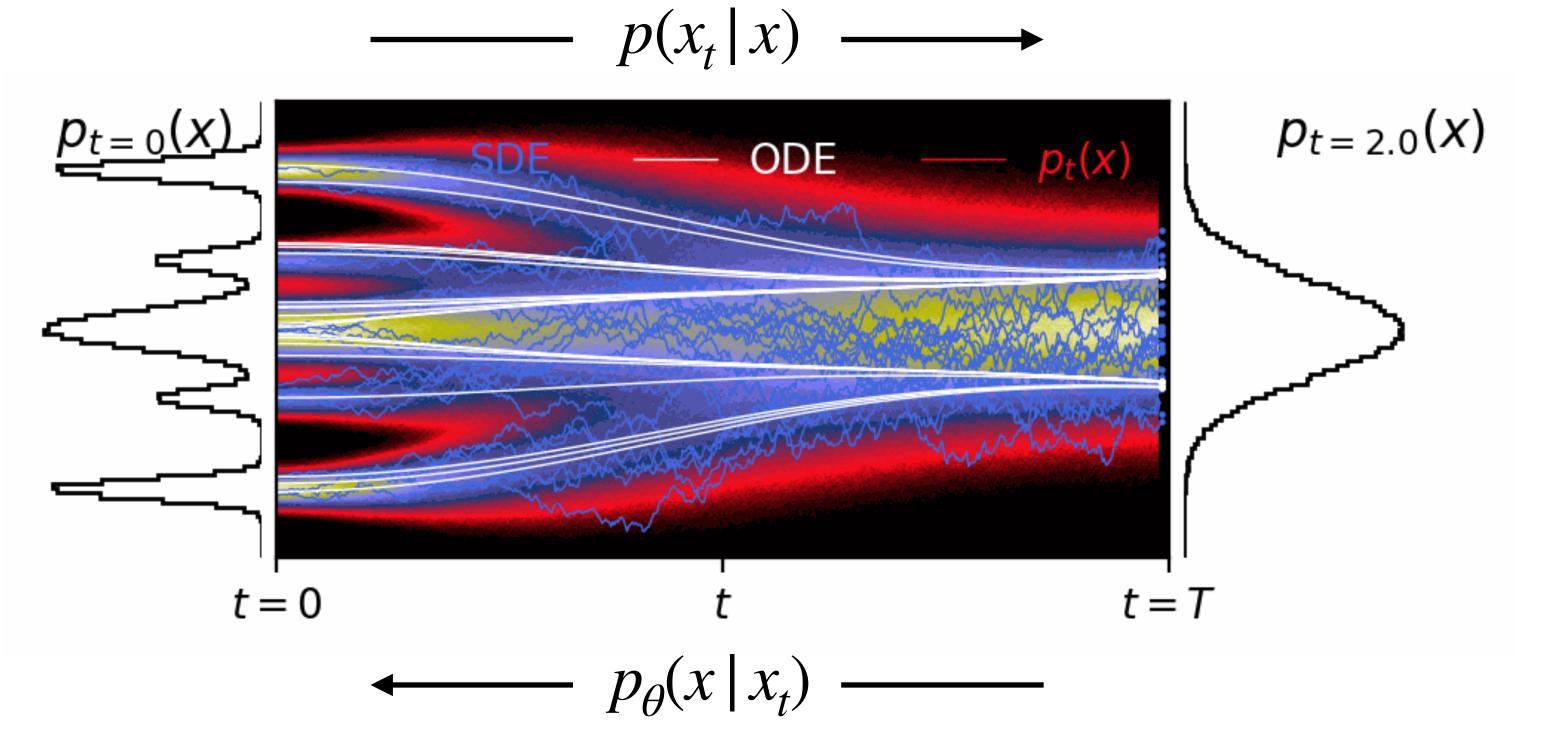
What quantifies a good prior p(x)?

• The evidence of the data given a prior p(x) and a likelihood $p(y \mid x)$

$$p(y) = \int dx \, p(y \mid x) p(x)$$

• What is a good parameterisation for p(x) given high-dimensional x?

Diffusion models: a form for p(x)





At each time t minimise

$$\theta^* = \min_{\theta} \mathbb{E}_x \left[\mathbb{E}_{x_t \mid x} \left[\| \nabla_{x_t} \log p(x \mid x_t) - \nabla_{x_t} \log p_{\theta}(x_t; t) \|_2^2 \right] \right]$$



How to fit to a model for p(x) given only y?

• This is a famously difficult task known as density deconvolution

- Extreme density deconvolution [Bovy++2009],
- AmbientDiffusion [Darras++2023, ++2024],
- Flow Density Deconvolution [Dockhorn++2020],
- Noise2NoiseFlow [Maleky++2022].

How to fit to a model for p(x) given only y?

Maximise the model evidence of the data given the model prior

$$\theta^* = \min_{\theta} \mathcal{D}_{KL}[p(y) \| p_{\theta}(y)]$$

• Expectation maximisation: guaranteed to monotonically increase over iterations

Expectation Maximisation

• Using samples $y \sim p(y)$, generate a training set for x to fit $p_{\theta}(x)$

$$\pi_k(x) = \int dy \, p_{\theta_k}(x \mid y) p(y)$$

Maximise the model evidence of the data given the model prior

$$\theta_{k+1} = \min_{\theta} \mathcal{D}_{KL}[\pi_k(x) \| p_{\theta}(x)]$$

Guaranteed to monotonically increase over iterations (local minimum)

Diffusion posterior sampling for x

• What is $p_{\theta}(x | y)$? Why do we need it?

• Given that our model $p(y \mid x)$ is analytic, we can sample $p_{\theta}(x \mid y)$ using Bayes

$$\nabla_{x_t} \log p(x_t | y) = \nabla_{x_t} \log p(y | x_t) + \nabla_{x_t} \log p(x_t)$$



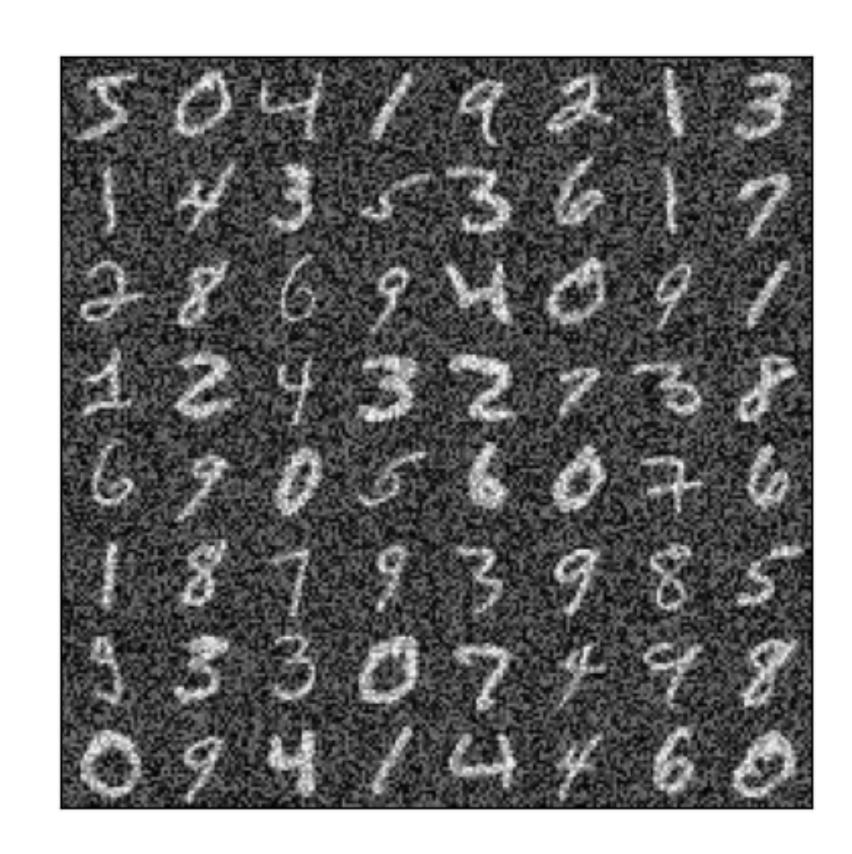
Algorithm

- dataset $\{y\}$ # dataset is fixed
- ullet initialise $heta_0$
- for k in 1:K:
 - -get batch y
 - sample $x | y, \theta_k$
 - minimise diffusion loss for x
 - update model parameters $heta_k$
- ullet return $heta_K$

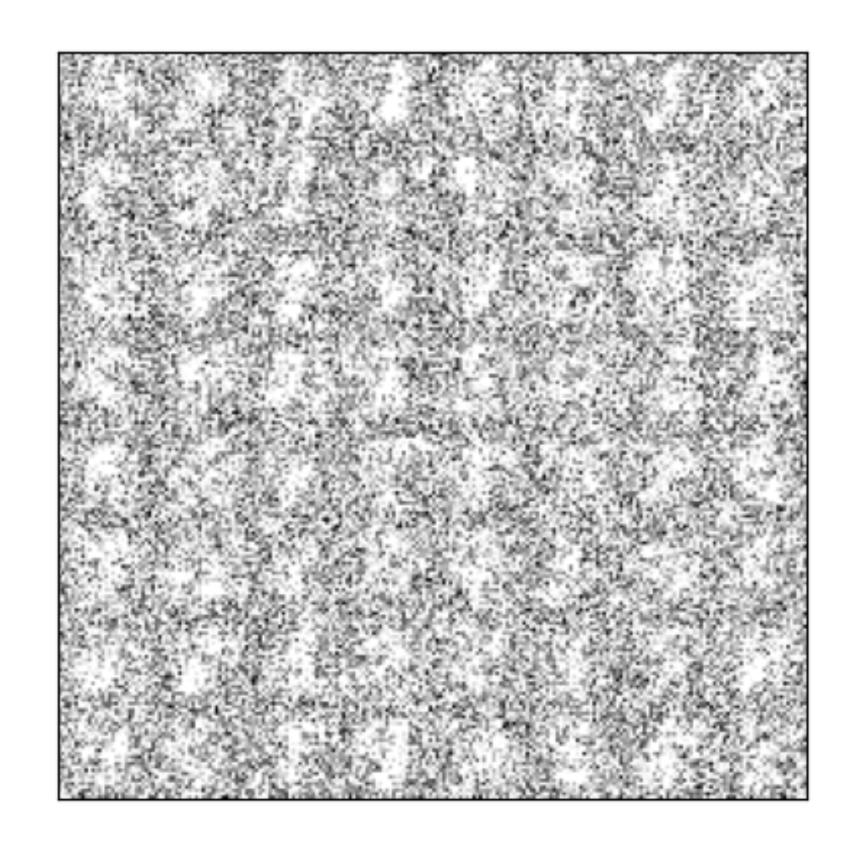


Example: MNIST

• 40 minutes of training, no GPU, transformer-based diffusion



$$y \sim \mathcal{G}[y \mid x, \Sigma_y]$$



$$x \sim p_{\theta}(x \mid y)$$



Details I did not cover

- Accurate diffusion posterior sampling
 - Bottleneck of this method

$$\nabla_{x_t} \log p(x_t | y) = \nabla_{x_t} \log p(y | x_t) + \nabla_{x_t} \log p(x_t)$$

• Only an approximation to this term exists...

$$q(y|x_t) = \int dx \, p(y|x)p(x|x_t) = \mathcal{G}[y|\mathbb{E}[x|x_t], \Sigma_y + \mathbb{V}[x|x_t]]$$

$$\Longrightarrow \nabla_{x_t} \log q(y \mid x_t) = \nabla_{x_t} \mathbb{E}[x \mid x_t]^{\mathsf{T}} \left(\Sigma + \mathbb{V}[x \mid x_t] \right)^{-1} \left(y - \mathbb{E}[x \mid x_t] \right)$$

• Express as Ax = b, **CG** solve to avoid calculating $\mathbb{V}[x \mid x_t] = \sum_t \nabla_{x_t}^T d_{\theta}(x_t, t)$