ELV: Embodied Learning and Vision

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NYU

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elvcourse.org

Module 1:
Deep Learning for Structured Outputs

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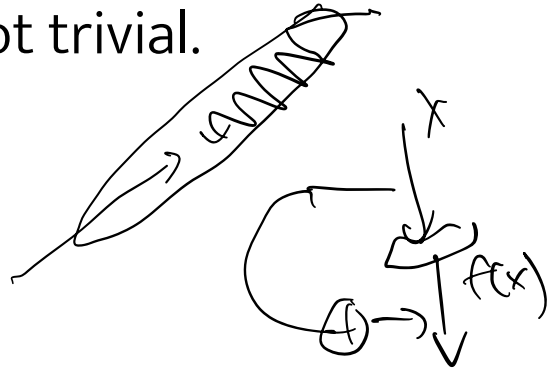
Deep Learning

- Over decades, optimizing deep neural networks was not trivial.

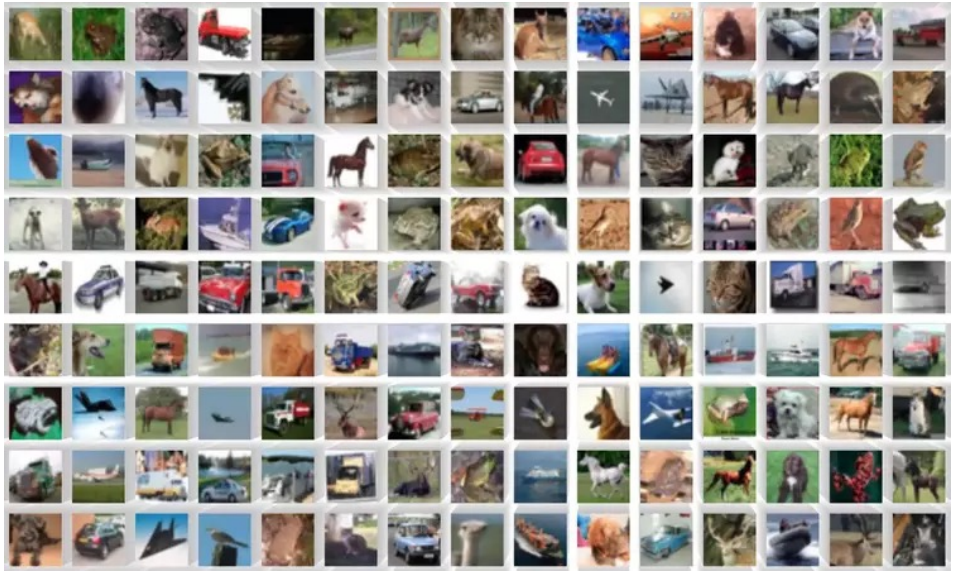
Deep Learning

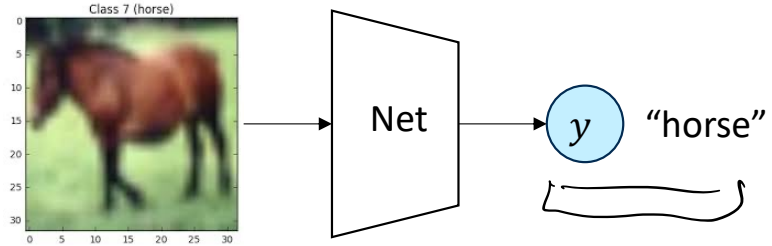
- Over decades, optimizing deep neural networks was not trivial.
- Progress came from (taken for granted nowadays):
  - Initialization
  - Optimizers (Adam, gradient conditioning)
  - Normalization (BN, LN, GN, etc.)
  - Skip connection (recurrent net, residual net, preserving gradients)
  - Regularization (dropout, noise, augmentation)
  - Attention (generalization, parallelization)



Classification

- To test how we can fit a deep neural network well, people have relied on simple benchmarks, such as image classification.





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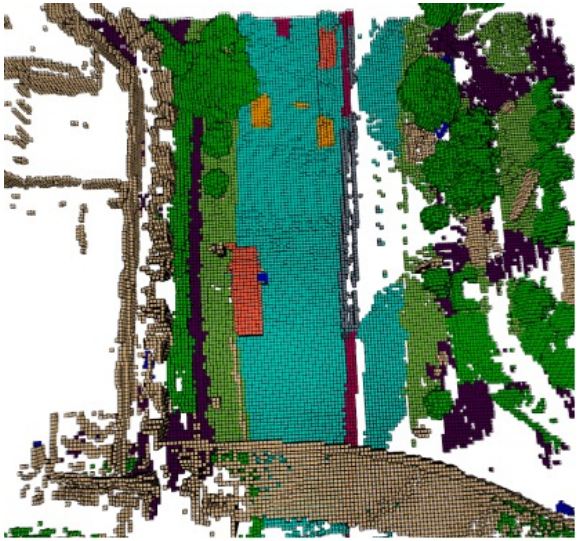
What are Structured Outputs?

- An embodied agent needs to have a structured output space.
  - Object localization, tracking, motion, spatial segmentation, 3d occupancy
  - Trajectory, forecasting, planning



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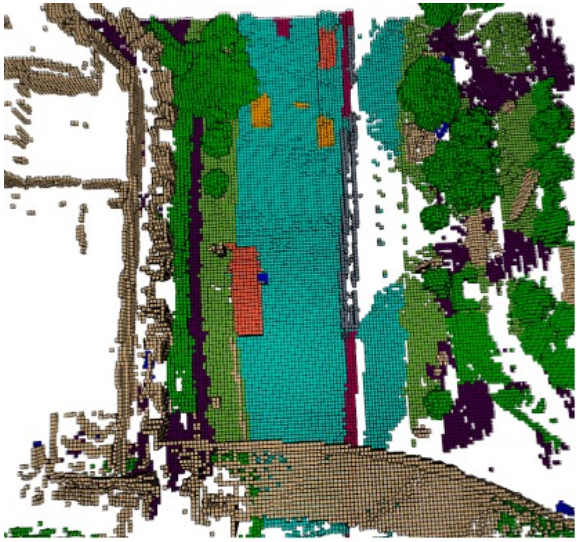

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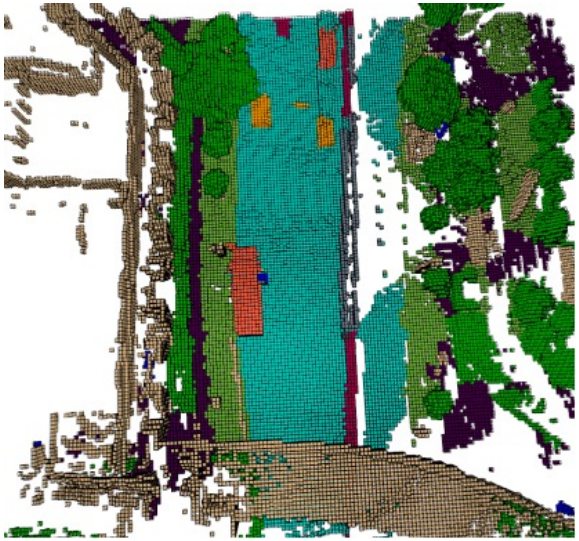

- It often does not reason the joint probability

$y = Wx$ (y_1) (y_2) (y_3) . (x)

$y_i = w_i^T x$

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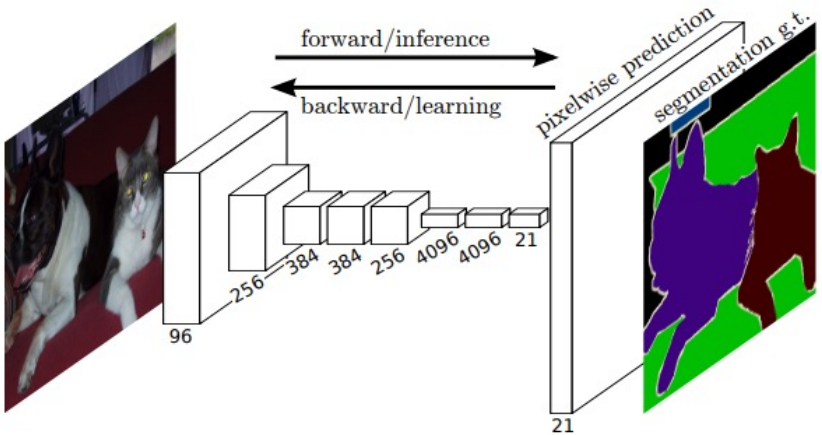
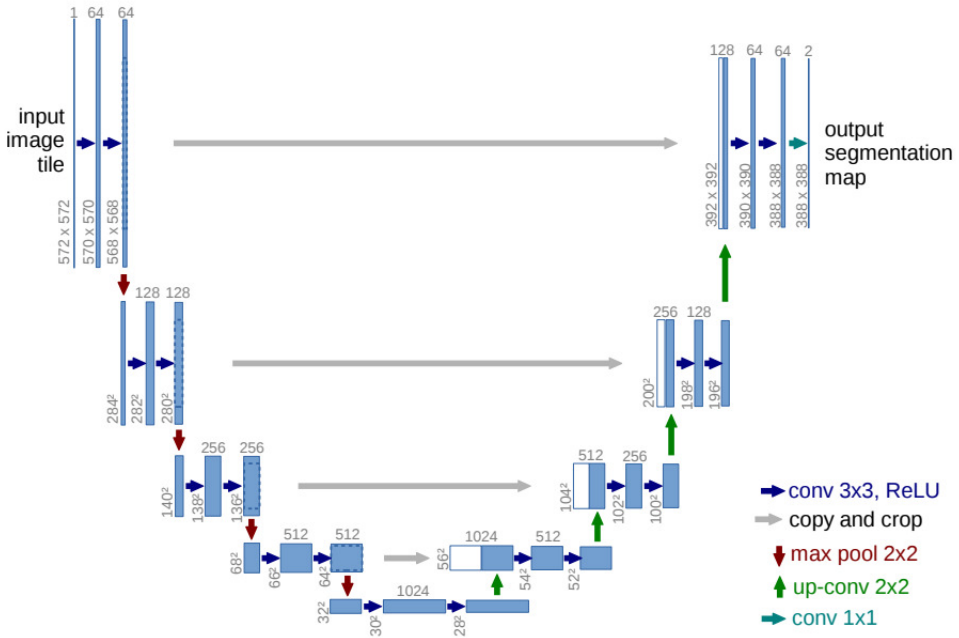
Network Architecture for Structured Outputs

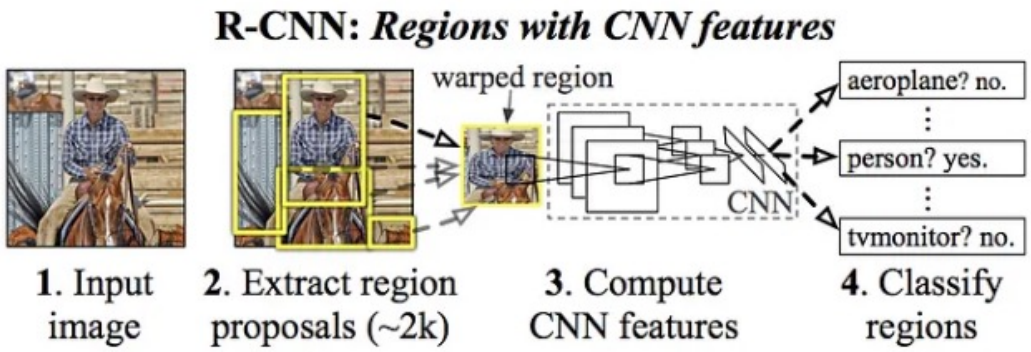
- Segmentation
- Spatial, high-resolution



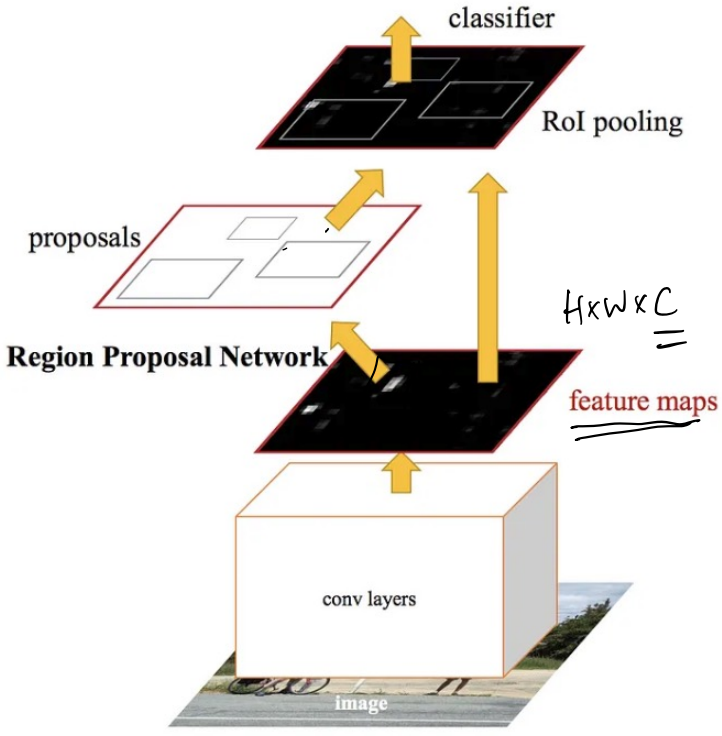


Network Architecture for Structured Outputs

- Object Detection



Girshick et al., 2013



Ren et al., 2015

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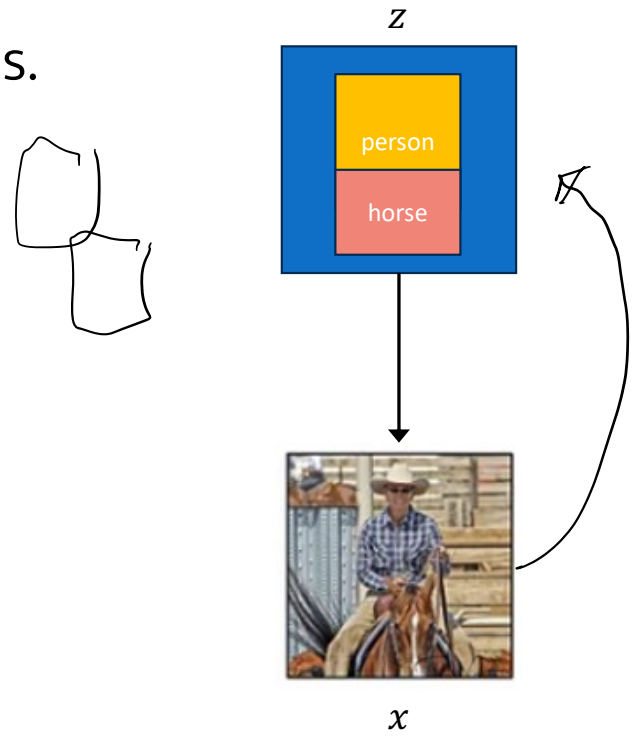
Object Detection as Inference

- Bounding boxes are structured latent variables.



Object Detection as Inference

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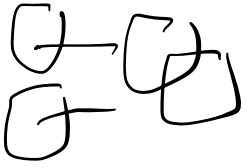

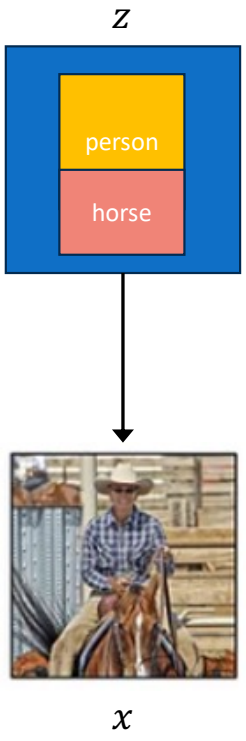

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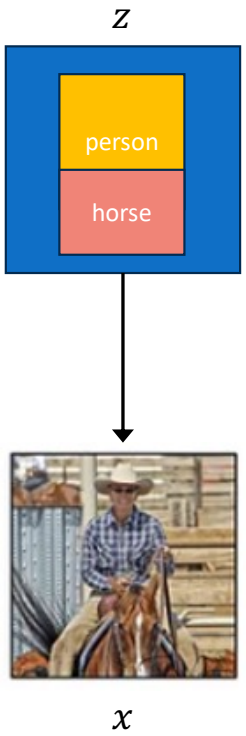
  - Context



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Object Detection as Inference

- Bounding boxes are structured latent variables.
- Occupancy as physical constraints.
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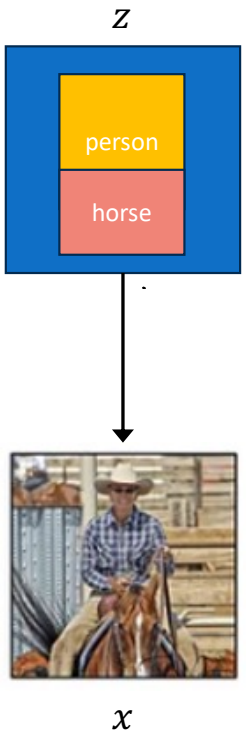
- The role of the network is to perform “inference” on the latent variables.



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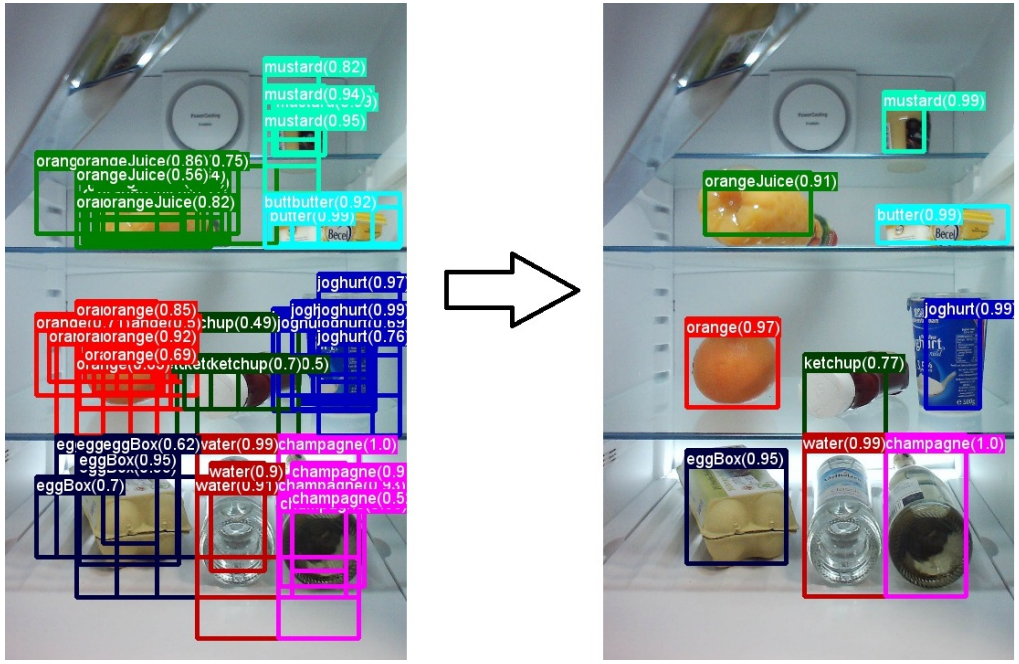
Non-Maximal Suppression

- Box Proposals: Samples of boxes that may come from a single object (latent)



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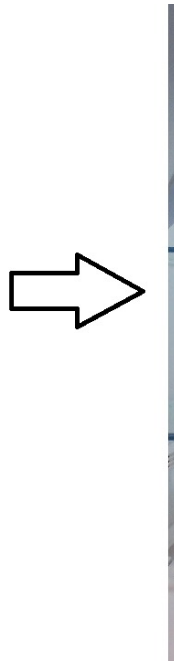
- Each with a confidence score, density representation of the inferred latent distribution $q(z|x)$.



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Non-Maximal Suppression

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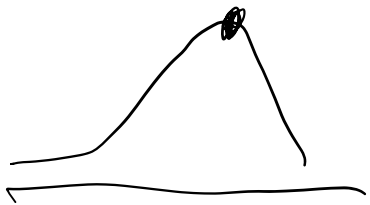
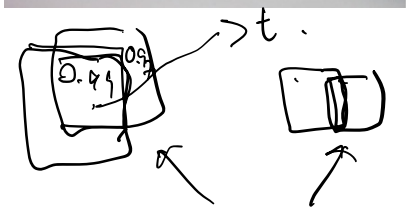
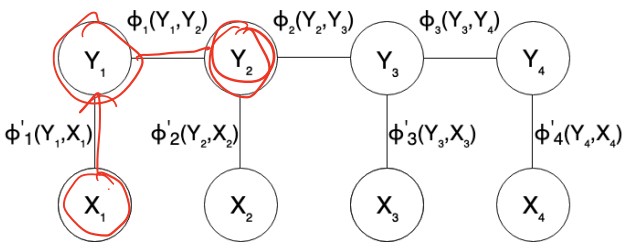
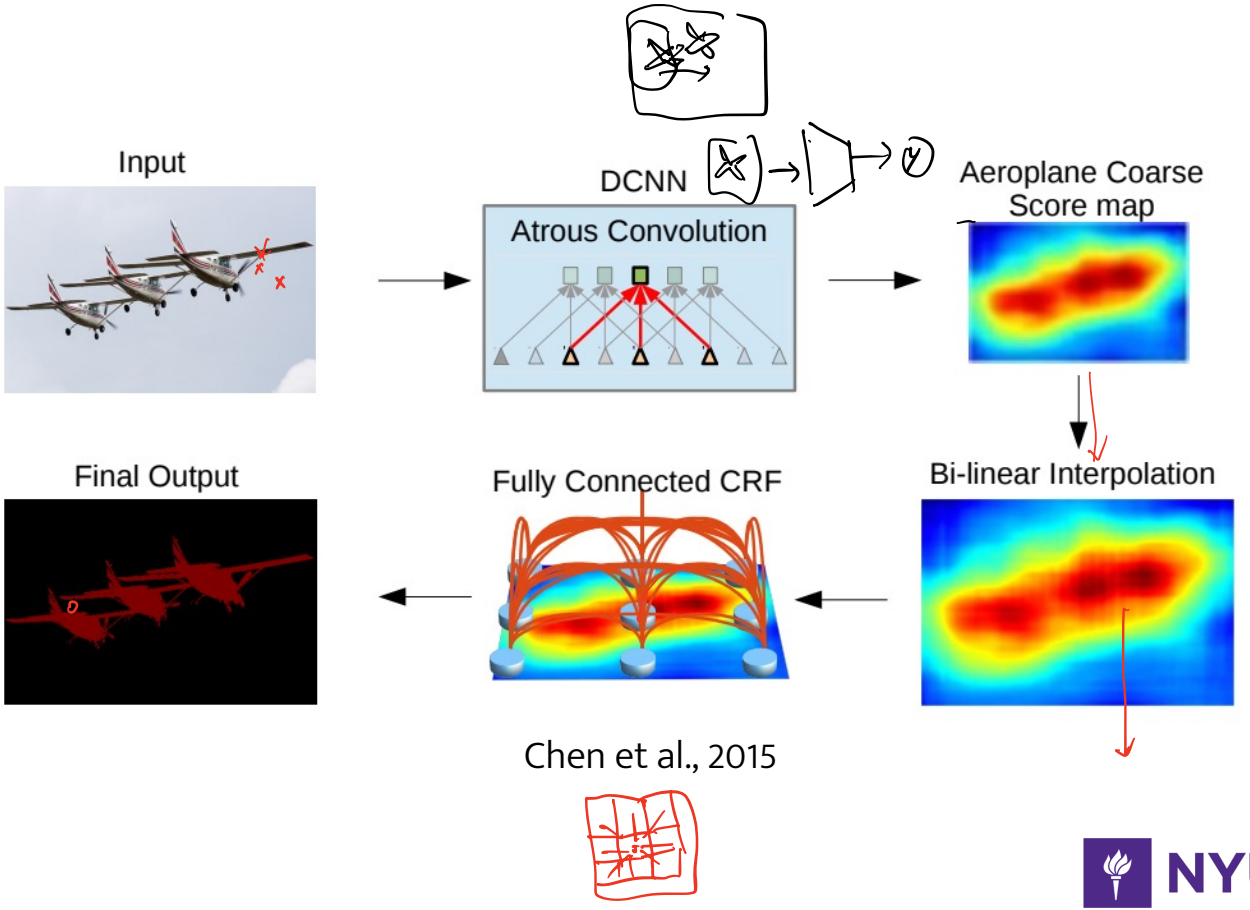
- MAP: take the mode of the distribution





Segmentation as CRF Inference





Chen et al., 2015

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Inference Problem

- Knows $p(x|z)$.

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$$p(z|x;\theta) = \frac{p(x,z;\theta)}{\int_z p(x,z;\theta)}.$$

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- Brute force

all possible latent state.

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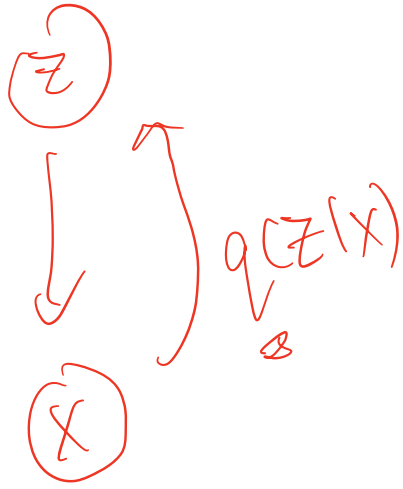

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- Stochastic sampling, MCMC

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Variational Inference

- Jensens inequality to get ELBO.

$$\log p(x) = \log \int_z p(x, z)$$

$$= \log \int_z p(x, z) \frac{q(z)}{q(z)}$$

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Variational Inference

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$$
\begin{aligned}
\log p(x) &= \log \int_z p(x,z) \\
&= \log \int_z p(x,z) \frac{q(z)}{q(z)} \\
&= \log \left(\mathbb{E}_q \frac{p(x,z)}{q(z)} \right) \\
&\geq \mathbb{E}_q \log \frac{p(x,z)}{q(z)} \\
&= \mathbb{E}_q \log p(x,z) - \mathbb{E}_q \log q(z) = \mathcal{L}.
\end{aligned}
$$

Mean-Field Inference

- If there are many latent variables, we can assume factorization (local variational approximation):

$$q(z_1, \ldots, z_m) = \prod_{j=1}^{m} q(z_j).$$

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$$q(z_1, \ldots, z_m) = \prod_{j=1}^{m} q(z_j).$$

$$\mathcal{L} = \log p(x) + \sum_{j=1}^{m} \mathbb{E}_{q(z_j)} \log p(z_j | z_{-j}, x) - \mathbb{E}_{q(z_j)} \log(q(z_j)).$$

Inference Operations

- CRF with pairwise energy. Use x as labels.

$$E(\mathbf{x}) = \sum_i \psi_u(x_i) + \sum_{i<j} \psi_p(x_i, x_j),$$

unary. binary.

[Krähenbühl & Koltun, 2012]

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$$\psi_p(x_i, x_j) = \mu(x_i, x_j) \underbrace{\sum_{m=1}^{K} w^{(m)} k^{(m)}(\mathbf{f}_i, \mathbf{f}_j)}_{k(\mathbf{f}_i, \mathbf{f}_j)}$$

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$$k^{(m)}(\mathbf{f}_i, \mathbf{f}_j) = \exp\left(-\tfrac{1}{2}(\mathbf{f}_i - \mathbf{f}_j)^{\mathrm{T}} \Lambda^{(m)} (\mathbf{f}_i - \mathbf{f}_j)\right)$$

$$w^{(1)} \underbrace{\exp\left(-\frac{|p_i - p_j|^2}{2\theta_\alpha^2} - \frac{|I_i - I_j|^2}{2\theta_\beta^2}\right)}_{\text{appearance kernel}} + w^{(2)} \underbrace{\exp\left(-\frac{|p_i - p_j|^2}{2\theta_\gamma^2}\right)}_{\text{smoothness kernel}}.$$

$$\mu(x_i, x_j) = [x_i \neq x_j]$$

[Krähenbühl & Koltun, 2012]

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Inference in Fully Connected CRF

- Iterative mean-field inference.

Algorithm 1 Mean field in fully connected CRFs

Initialize Q ▷ $Q_i(x_i) \leftarrow \frac{1}{Z_i}\exp\{-\phi_u(x_i)\}$

while not converged **do** ▷ See Section 6 for convergence analysis

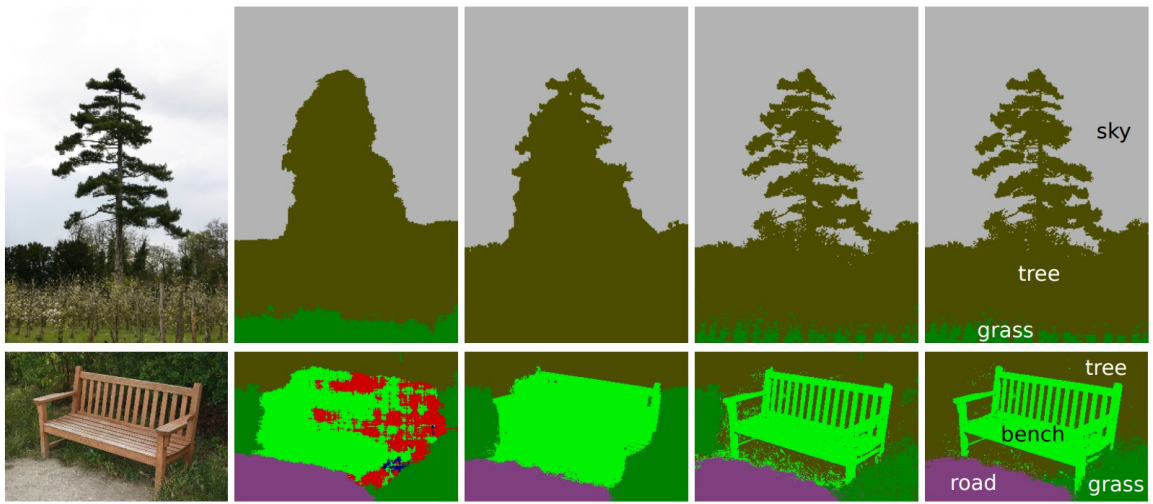
$\tilde{Q}_i^{(m)}(l) \leftarrow \sum_{j \neq i} k^{(m)}(\mathbf{f}_i, \mathbf{f}_j) Q_j(l)$ for all m ▷ **Message passing** from all X_j to all X_i

$\hat{Q}_i(x_i) \leftarrow \sum_{l \in \mathcal{L}} \mu^{(m)}(x_i, l) \sum_m w^{(m)} \tilde{Q}_i^{(m)}(l)$ ▷ **Compatibility transform**

$Q_i(x_i) \leftarrow \exp\{-\psi_u(x_i) - \hat{Q}_i(x_i)\}$ ▷ **Local update**

normalize $Q_i(x_i)$

end while



(a) Image (b) Unary classifiers (c) Robust P^n CRF (d) Fully connected CRF, MCMC inference, 36 hrs (e) Fully connected CRF, our approach, 0.2 seconds

[Krähenbühl & Koltun, 2012]

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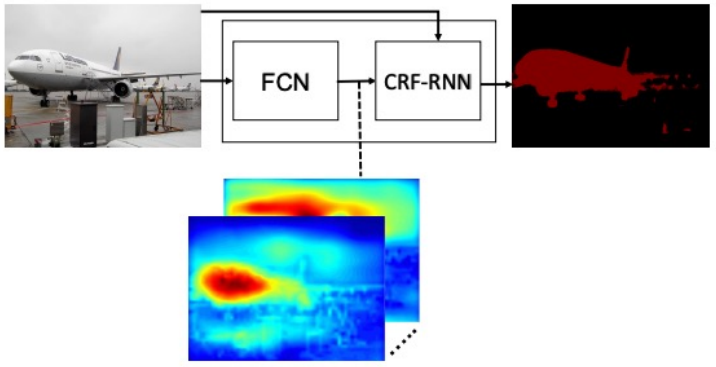
CRFs as RNNs



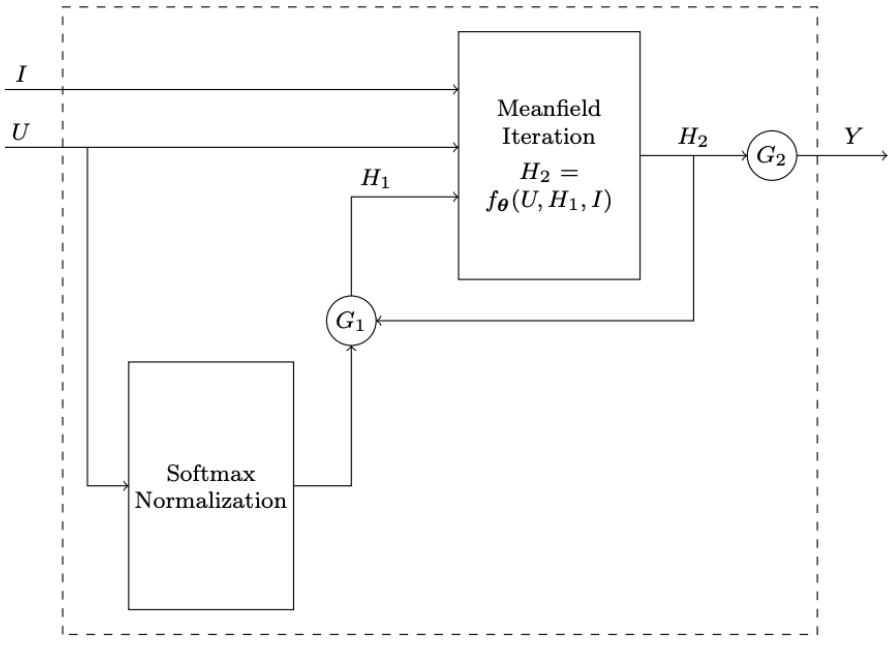


Figure 2. **The CRF-RNN Network.** We formulate the iterat mean-field algorithm as a Recurrent Neural Network (RNN). G ing functions G_1 and G_2 are fixed as described in the text.

$Q_i(l) \leftarrow \frac{1}{Z_i} \exp\left(U_i(l)\right)$ for all i ▷ Initialization

while not converged **do**

$\tilde{Q}_i^{(m)}(l) \leftarrow \sum_{j \neq i} k^{(m)}(\mathbf{f}_i, \mathbf{f}_j) Q_j(l)$ for all m

▷ Message Passing

$\check{Q}_i(l) \leftarrow \sum_m w^{(m)} \tilde{Q}_i^{(m)}(l)$

▷ Weighting Filter Outputs

$\hat{Q}_i(l) \leftarrow \sum_{l' \in \mathcal{L}} \mu(l, l') \check{Q}_i(l')$

▷ Compatibility Transform

$\breve{Q}_i(l) \leftarrow U_i(l) - \hat{Q}_i(l)$

▷ Adding Unary Potentials

$Q_i \leftarrow \frac{1}{Z_i} \exp\left(\breve{Q}_i(l)\right)$

▷ Normalizing

end while

[Zheng et al., 2015]

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Summary

- Perception of high dimensional objects can be viewed as inferring latent variables with probabilistic distributions.

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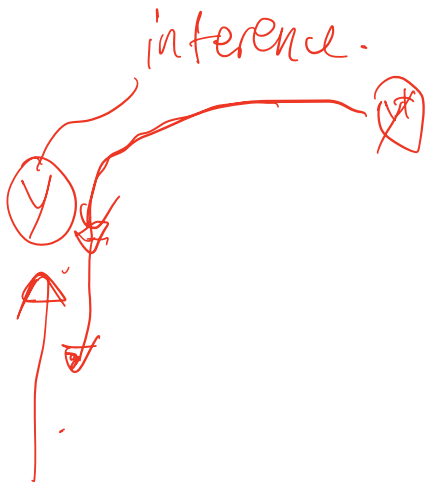
- Perception of high dimensional objects can be viewed as inferring latent variables with probabilistic distributions.
- We can impose structure.
- We can learn through the inference process.
  - Taking the inference process into account.
  - Learning representations that matter.



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Some Nuances

- If the process is deterministic or unimodal, standard deep networks may work.

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Some Nuances

- If the process is deterministic or unimodal, standard deep networks may work.
- Network forward propagation vs. relaxed probabilistic inference.
- Having a stronger prior has the potential to be more data efficient.
- And you will need structured / generative learning when there are multiple modes.
  - E.g. Motion generation and planning: there can be multiple future trajectories

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Deep Generative Models

- Autoregressive models

Deep Generative Models

- Autoregressive models
- Energy-based models
  - CRF
  - Max-Margin

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Deep Generative Models

- Autoregressive models
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- Normalizing flow

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Deep Generative Models

- Autoregressive models
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  - CRF
  - Max-Margin
- Normalizing flow
- Diffusion models

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Autoregressive Modeling

- Another type of output is autoregressive modeling.

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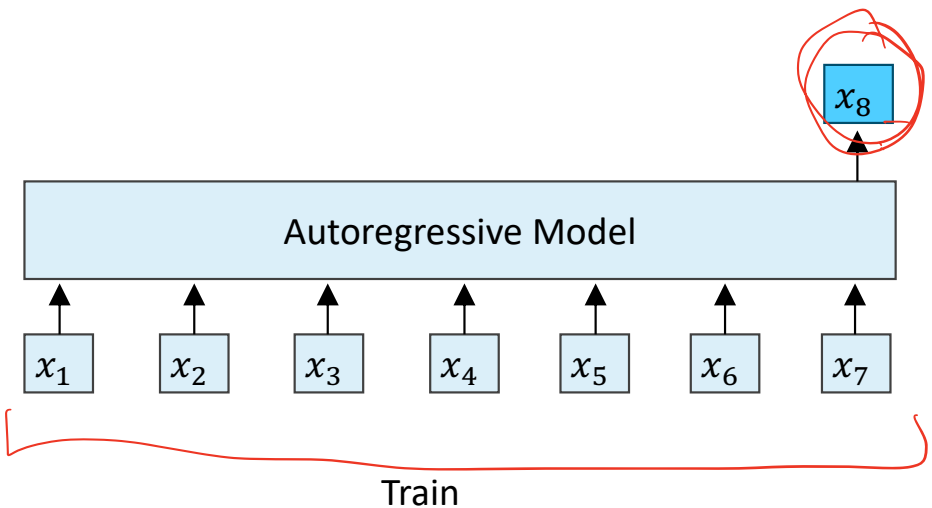
- Example: Object detection/segmentation.

Autoregressive Modeling

- Another type of output is autoregressive modeling.
- Example: Object detection/segmentation.
- Intuition: Our visual attention focus on one object at a time.

Teacher Forcing

- Teacher Forcing: Pretend that you know the whole sequence $\{y_1 \ldots y_t\}$ at training time, and train for y_{t+1}.



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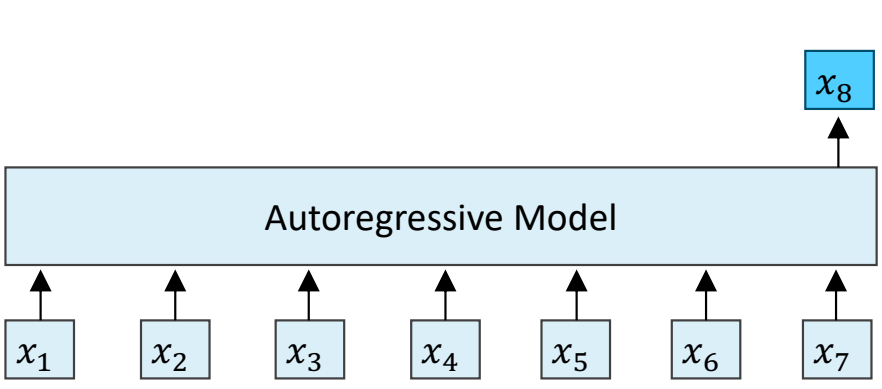
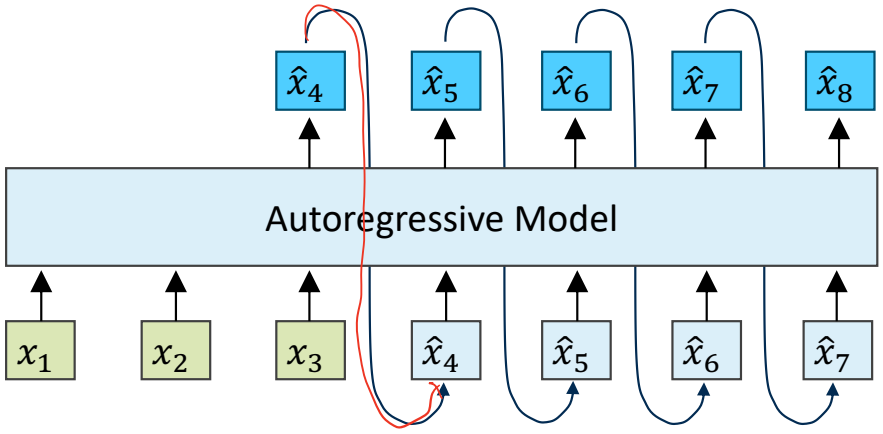


Train



Test

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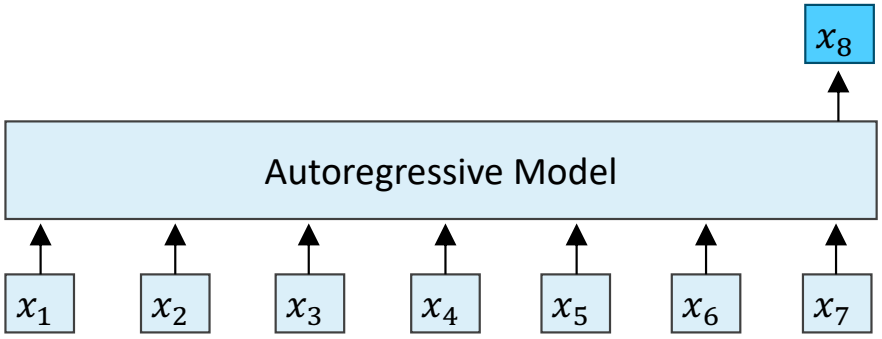
Teacher Forcing

- Teacher Forcing: Pretend that you know the whole sequence $\{y_1 \ldots y_t\}$ at training time, and train for y_{t+1}.
- Problem: You have to know the ordering.



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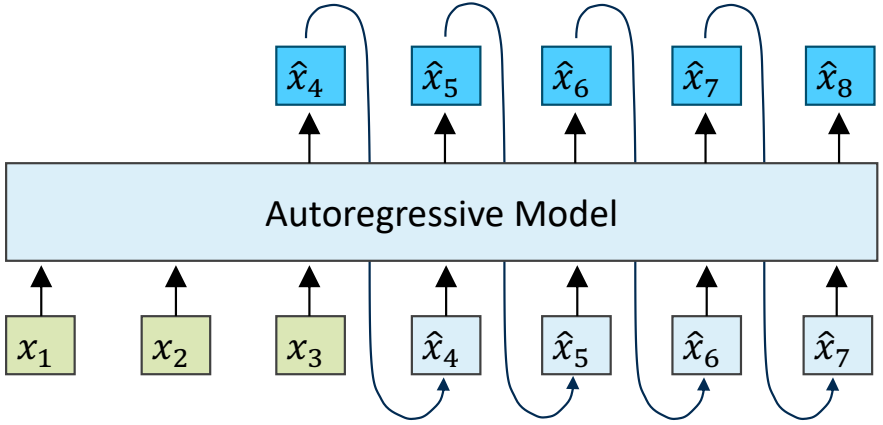

Test

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More on Ordering

- There are many set to set problems.

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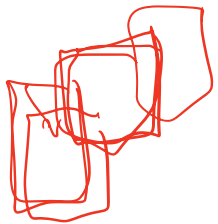
- E.g. Detection, segmentation, generating multiple objects, clustering



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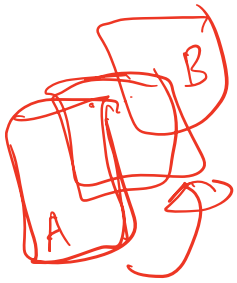
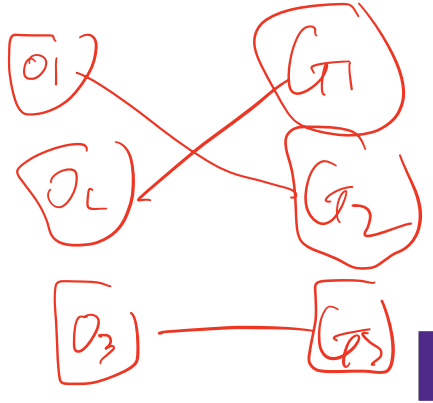
More on Ordering

- There are many set to set problems.
- E.g. Detection, segmentation, generating multiple objects, clustering
- Input does not follow a particular order. Loss function should not favor a particular order.
  - Attention: The attention operation is order-invariant.
  - Matching: The teacher can match the next input based on the closest matching ground truth instances.





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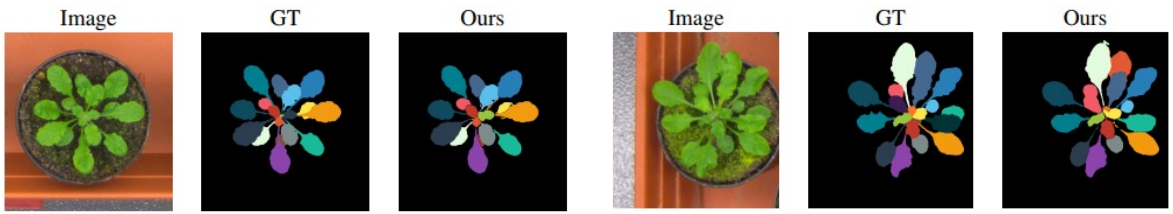
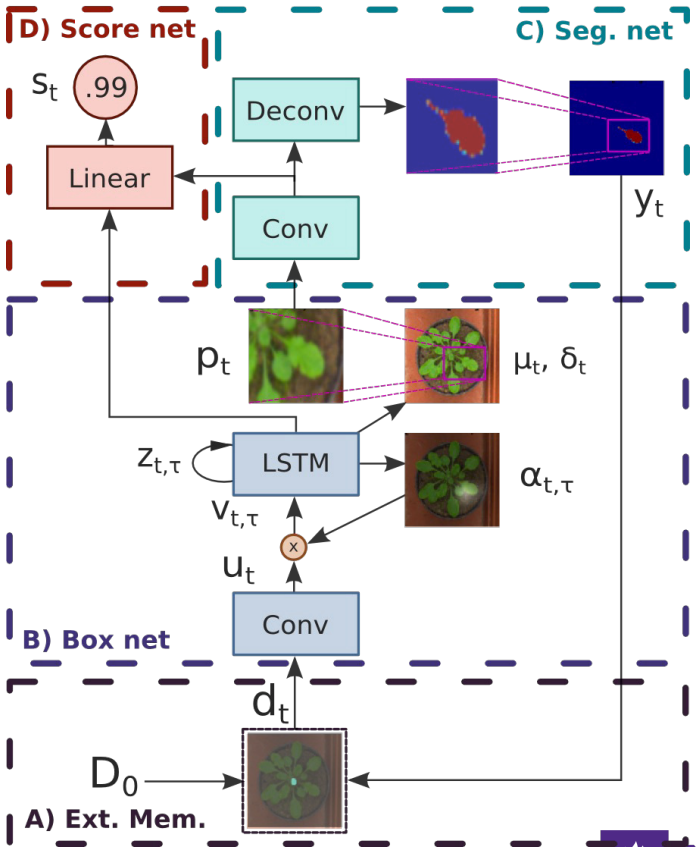
Instance Segmentation using Attention

- Attending to one region at a time.
- Zooming in for segmentation.
- End-to-end differentiable box proposals and external memory.
- State-of-the-art on leave segmentation problems for many years.





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Summary

- Autoregressive models
  - Exact likelihood (instead of a lower bound or approximation)
  - Conditional probability may be easier to model
  - Need an ordering
  - Can take a long time to decode

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- Generating the next variable is a different objective from learning a good representation of the whole sequence.
- No hierarchical planning.

Energy-Based Modeling

- The goal is to learn a distribution $p(x)$ to model the set of examples.

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Energy-Based Modeling

- The goal is to learn a distribution $p(x)$ to model the set of examples.
- Assuming Boltzmann distribution:

$$p(x;\theta) = \frac{1}{Z(\theta)} \exp(-E(x;\theta))$$

$$Z(\theta) = \int_X \exp(-E(x;\theta))$$

network.

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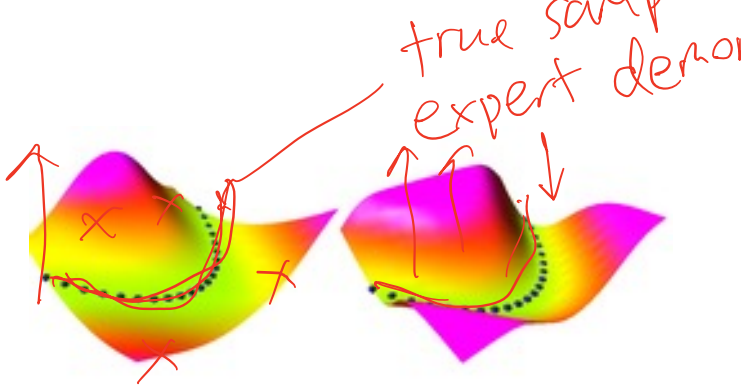


Picture from LeCun

- Maximizing the likelihood:

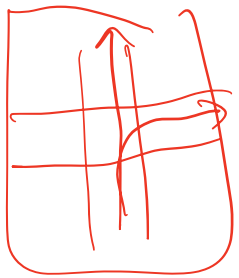
$$\frac{\partial}{\partial\theta} \log p(x;\theta) = \mathbb{E}_{x' \sim p(x)} \left[\frac{\partial E(x';\theta)}{\partial\theta} \right] - \frac{\partial E(x;\theta)}{\partial\theta}.$$

real data.

Structured Prediction

- EBM can be easily adapted to model the joint distribution of x and y.
- Requires optimization of y at inference time.

$$\arg\min_y E(x, y)$$



traj : y.

visual scene : x.

Optimization

- Computing $\mathbb{E}_{x' \sim p(x)} \left[\frac{\partial E(x';\theta)}{\partial \theta} \right]$ is non-trivial. We need to sample from p(x).

Song & Kingma. How to Train Your Energy-Based Models.

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- But we only know $E(x)$!
- Through MCMC samplers: MH, Langevin, HMC, Gibbs.
- Approximations: Using truncated steps (Contrastive Divergence)
- Score Matching: Tries to model the score function $\nabla_x \log p_\theta(x)$
  - If we know the gradient, we can improve the samples.
  - Want the model gradient to match with that from the data distribution
  - Closely related to diffusion models

Song & Kingma. How to Train Your Energy-Based Models.

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Max-Entropy Inverse RL

- Want to model the reward function of trajectories.
- Given a reward function, the policy distribution can be modeled as a Boltzmann distribution.
- Given expert trajectories, we can maximize the likelihood under such distribution induced by the learned reward

$$p(\tau|\mathcal{O}_{1:T},\psi) \propto \cancel{p(\tau)} \exp\left(\sum_t r_\psi(\mathbf{s}_t,\mathbf{a}_t)\right)$$

can ignore (independent of ψ)

maximum likelihood learning: $$\max_\psi \frac{1}{N}\sum_{i=1}^{N} \log p(\tau_i|\mathcal{O}_{1:T},\psi) = \max_\psi \frac{1}{N}\sum_{i=1}^{N} r_\psi(\tau_i) - \log Z$$

Slide credit: Sergey Levine

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Max-Entropy Inverse RL

$$\max_{\psi} \frac{1}{N} \sum_{i=1}^{N} r_\psi(\tau_i) - \log Z \qquad Z = \int p(\tau) \exp(r_\psi(\tau)) d\tau$$

$$\nabla_\psi \mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} \nabla_\psi r_\psi(\tau_i) - \underbrace{\frac{1}{Z} \int p(\tau) \exp(r_\psi(\tau)) \nabla_\psi r_\psi(\tau) d\tau}_{p(\tau|\mathcal{O}_{1:T}, \psi)}$$

current policy.

$$\nabla_\psi \mathcal{L} = E_{\tau \sim \pi^\star(\tau)}[\nabla_\psi r_\psi(\tau_i)] - E_{\tau \sim p(\tau|\mathcal{O}_{1:T}, \psi)}[\nabla_\psi r_\psi(\tau)]$$

estimate with expert samples

soft optimal policy under current reward

Slide credit: Sergey Levine

Ziebart et al. Maximum Entropy Inverse Reinforcement Learning. AAAI 2008.

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Max-Margin Learning

- In addition to probabilistic learning, we can also apply the max-margin framework.

Max-Margin Learning

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- Review: SSVM vs. CRF.

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$$\arg\min_\theta \sum_{n=1}^{N} \max[0, m + E(x_n;\theta) - E(x^*;\theta)] + \lambda||\theta||_2^2.$$

n^{th} demo

best output from model.

Max-Margin Learning

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- Review: SSVM vs. CRF.

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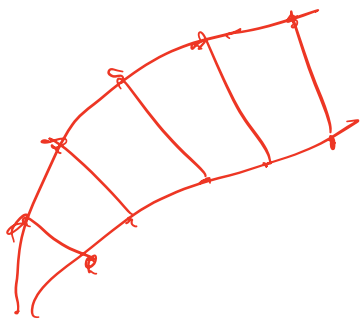
- Margin can be difference in trajectories.



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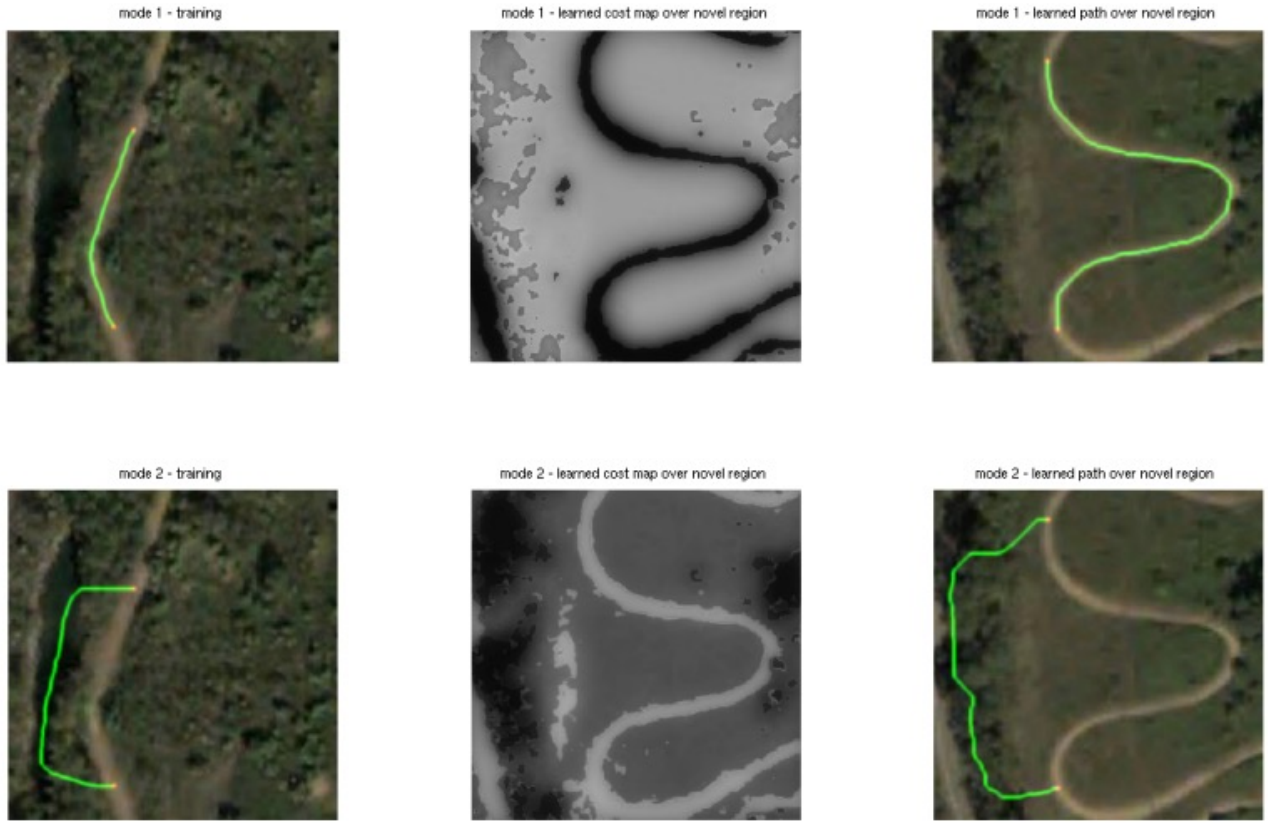
- Margin can be difference in trajectories.
- Non-probabilistic
- Still need to run optimization to find the best x^*

Samples

Max-Margin Planning



Ratliff et al. Maximum Margin Planning. ICML 2006.

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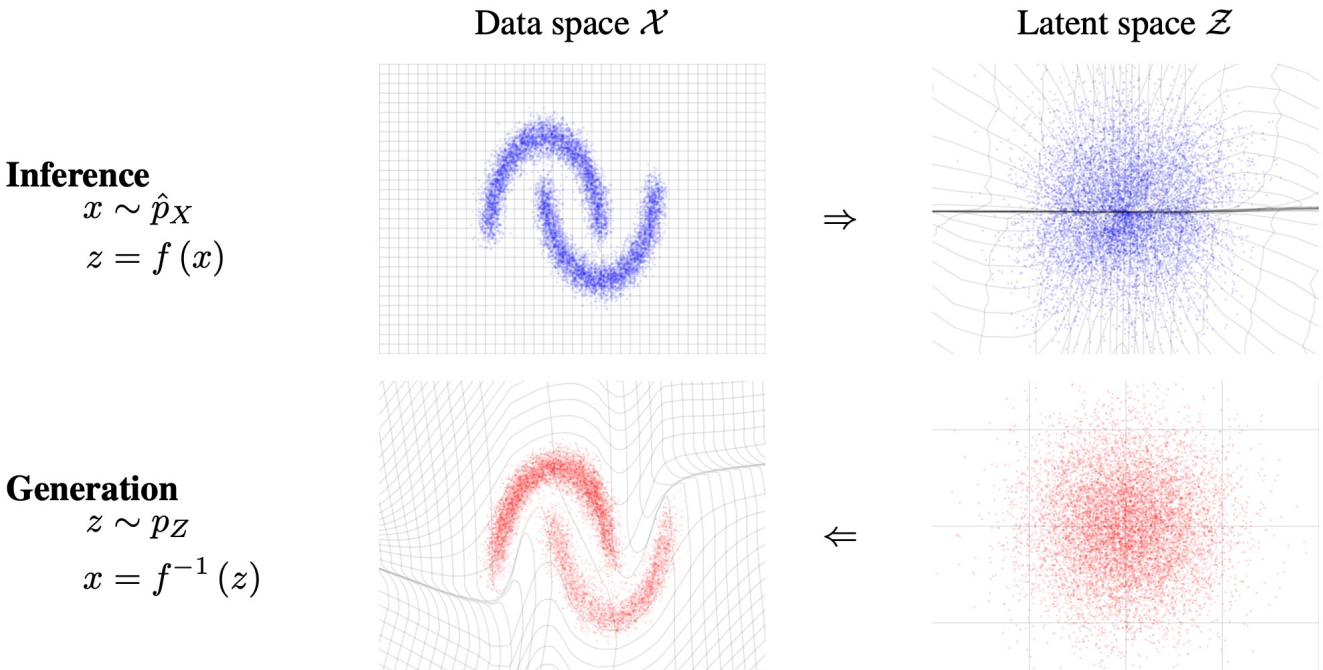
Learning Latent Representations

- z may contain useful high-level compressed information of the input.



Variational Autoencoders (VAE)

- z from a simple prior distribution.
- Optimize ELBO.

$$\log p_\theta(\mathbf{x}) = \log \int p_\theta(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z}$$

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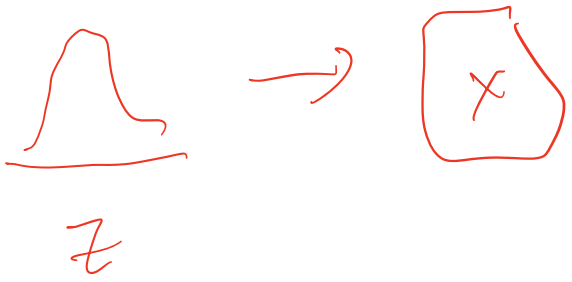

$$\log p_\theta(\mathbf{x}) = \log \int p_\theta(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z}$$

$$= \log \int \frac{q_\phi(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})} p_\theta(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z}$$

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$$\geq -\mathbb{D}_{\mathrm{KL}}[q_\phi(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})] + \mathbb{E}_q[\log p_\theta(\mathbf{x}|\mathbf{z})]$$

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VAE Problems

- Hard to transform the inputs to the prior distribution with a network.
- The coarser the approximation of q, the worse the lower bound.

$$
\begin{aligned}
ELBO &= \int_z q(z) \log \frac{p(x,z)}{q(z)} \\
&= \mathbb{E}_{q(z)} \log \frac{p(z|x)p(x)}{q(z)}
\end{aligned}
$$

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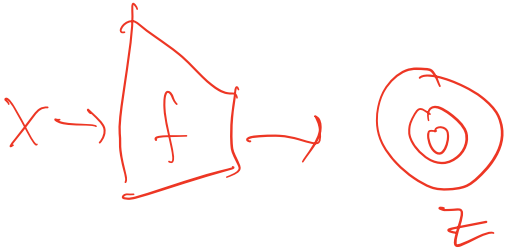

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&= -\mathbb{E}_{q(z)} \log \frac{q(z)}{p(z|x)} + \mathbb{E}_{q(z)} \log p(x) \\
&= -KL(q(z)||p(z|x)) + \log p(x)
\end{aligned}
$$

true posterior.

Normalizing Flows

- Requires a bijection between the input and output.

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$$\max_{\theta} \mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}} \log p_{\text{NF}}(\boldsymbol{x}; \theta) = \log p_0(f_\theta(\boldsymbol{x}); \theta) + \log \left(\left| \det \left(\frac{\partial f_\theta(\boldsymbol{x})}{\partial \boldsymbol{x}} \right) \right| \right)$$

Normalizing Flows

- Requires a bijection between the input and output.
- Needs to maintain dimensionality.
- Needs an efficient way to estimate determinant of Jacobian (typically O(n^3)).

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Adding Constraints in Transformation

- Rezende & Mohamed (2015):

$$f(\boldsymbol{z}) = \boldsymbol{z} + \boldsymbol{u}h(\boldsymbol{w}^\top \boldsymbol{z} + b).$$

Rezende & Mohamed. Variational Inference with Normalizing Flows. ICML 2015.

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Adding Constraints in Transformation

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scalar

parameter.

- Determinant of Jacobian:

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$$\left|\det \frac{\partial f}{\partial \boldsymbol{z}}\right| = |\det(I + \boldsymbol{u}\psi(\boldsymbol{z})^\top)| = |1 + \boldsymbol{u}^\top \psi(\boldsymbol{z})|.$$

Rezende & Mohamed. Variational Inference with Normalizing Flows. ICML 2015.

Masked Autoregressive Flow (MAF)

- Another way to make Jacobian determinant computable -> Lower triangular matrix.

Papamakarios et al. Masked Autoregressive Flow for Density Estimation. NIPS 2017.

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Masked Autoregressive Flow (MAF)

- Another way to make Jacobian determinant computable -> Lower triangular matrix.
- Consider the autoregression of generating one dimension at a time.

$$x_i = \mu_i(x_{1:i-1}) + \sigma_i(x_{1:i-1}) z_i, \quad z_i = \frac{x_i - \mu_i(x_{1:i-1})}{\sigma_i(x_{1:i-1})}.$$

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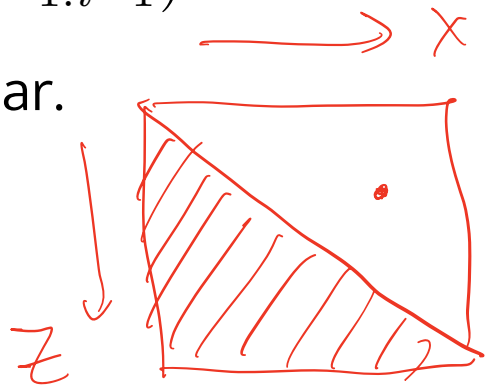

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$$\log|\det J| = \sum_{i=1}^{D} \log\left|\frac{1}{\sigma_i(x_{1:i-1})}\right| = -\sum_{i=1}^{D} \log \sigma_i(x_{1:i-1})$$

$$L = \sum_i \frac{1}{2}||z_i||_2^2 - \sum_i \log \sigma_i.$$

Papamakarios et al. Masked Autoregressive Flow for Density Estimation. NIPS 2017.

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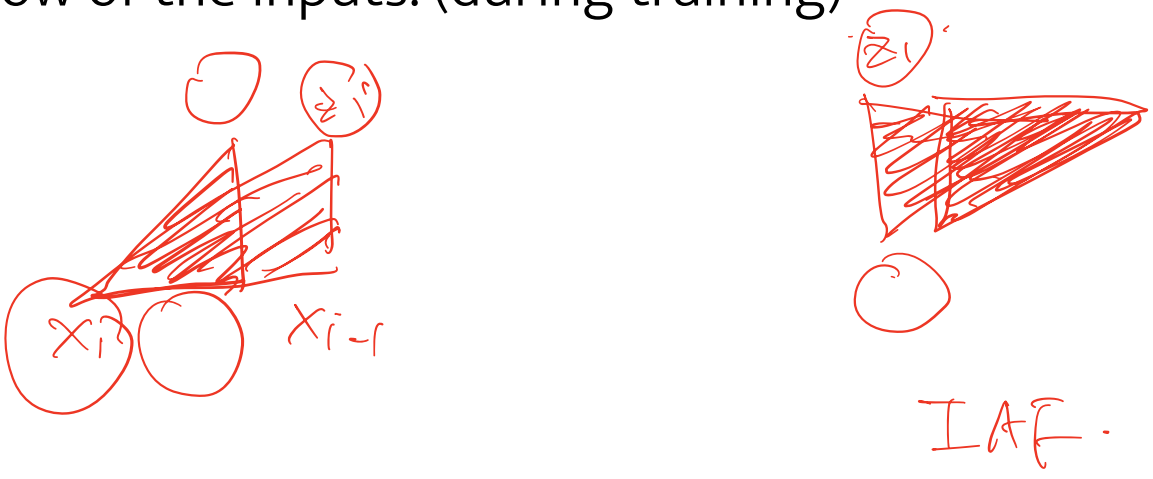
MAF vs IAF

- MAF inference can be parallelized by directly passing different window of the inputs. (during training)



Kingma et al. Improving Variational Inference with Inverse Autoregressive Flow. NIPS 2016.

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MAF vs IAF

- MAF inference can be parallelized by directly passing different window of the inputs. (during training)
- Sampling needs to be sequential: One input dimension at a time.
- Inverse Autoregressive Flow (IAF) does the reverse. Parallel sample, sequential inference (slow training).

Kingma et al. Improving Variational Inference with Inverse Autoregressive Flow. NIPS 2016.

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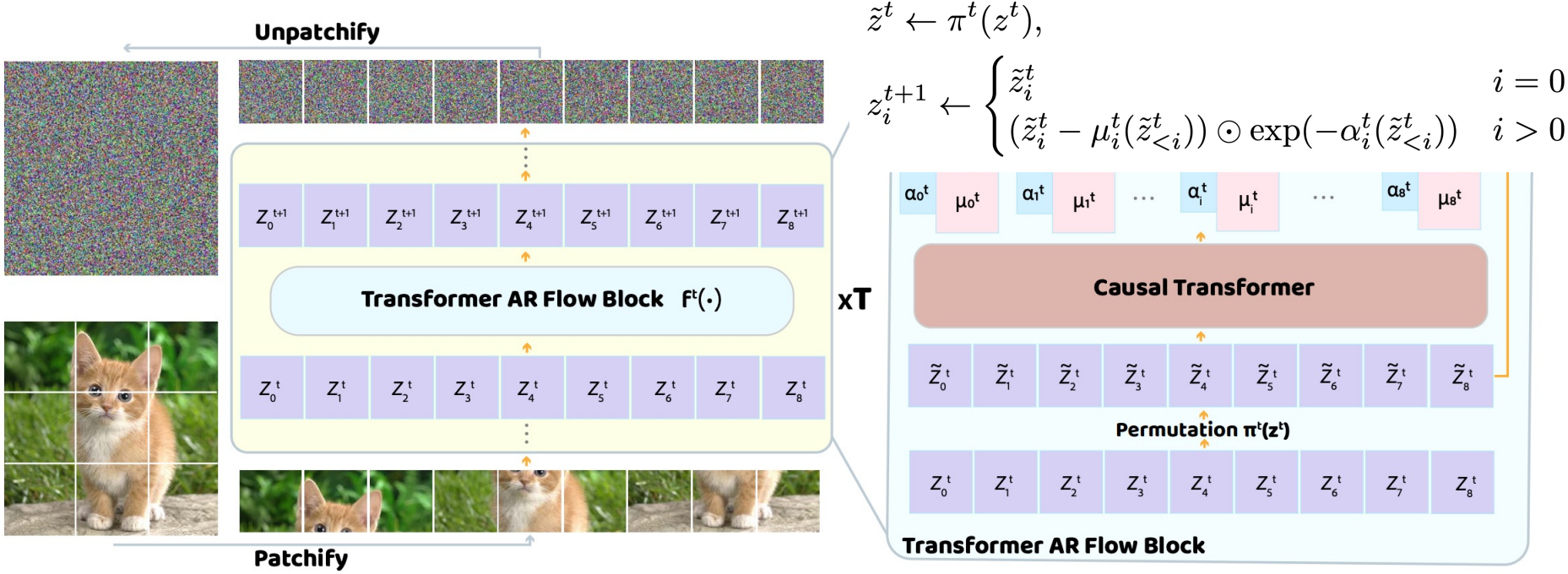
Block Autoregressive Flows

- Using blocks, permutations, and element-wise operations



$$\tilde{z}^t \leftarrow \pi^t(z^t),$$

$$z_i^{t+1} \leftarrow \begin{cases} \tilde{z}_i^t & i = 0 \\ (\tilde{z}_i^t - \mu_i^t(\tilde{z}_{<i}^t)) \odot \exp(-\alpha_i^t(\tilde{z}_{<i}^t)) & i > 0 \end{cases}$$

Zhai et al. Normalizing Flows are Capable Generative Models. ICML 2025.

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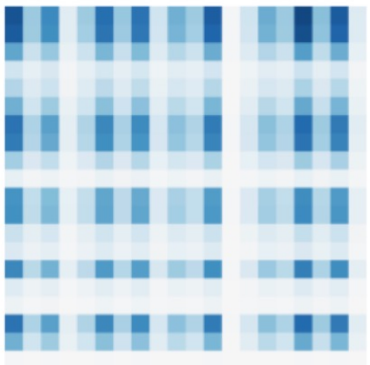
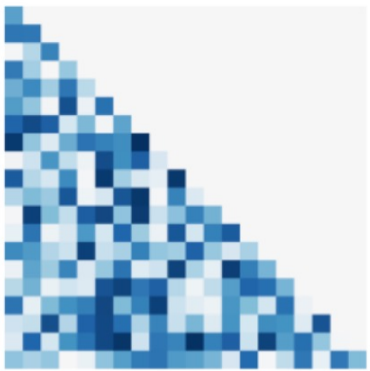
Full-Rank Jacobian

- Is it possible to make the architecture more flexible?



Low-rank



Auto-regressive

Full-rank

Image Credit

Behrmann et al. Invertible Residual Networks. ICML 2019.

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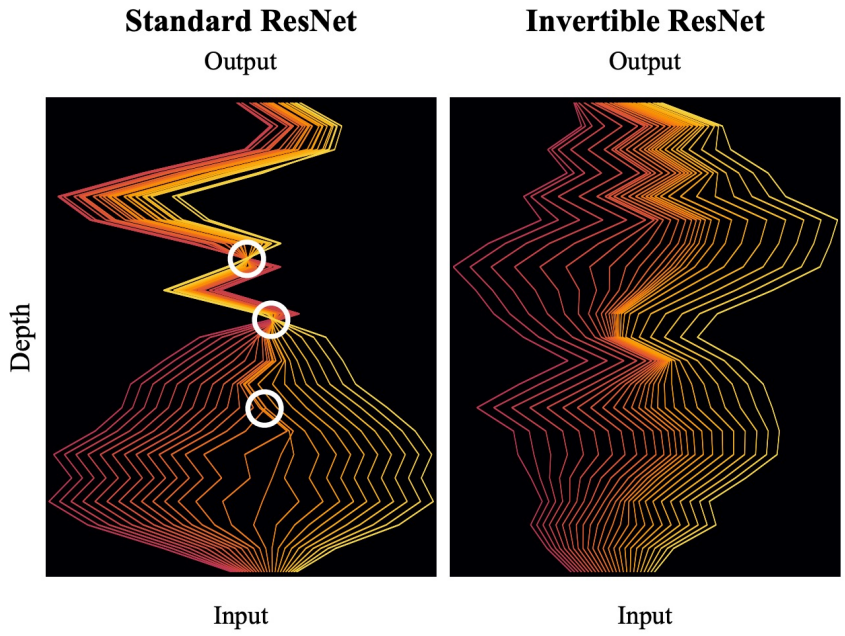
Invertibility of ResNet

$$x_{t+1} \leftarrow x_t + g_{\theta_t}(x_t)$$



Behrmann et al. Invertible Residual Networks. ICML 2019.

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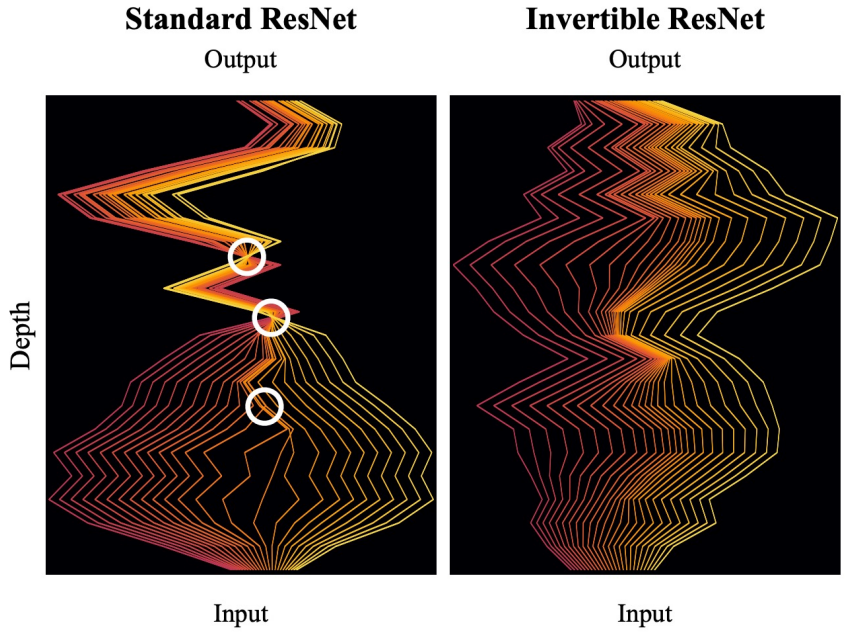
Invertibility of ResNet

$$x_{t+1} \leftarrow x_t + g_{\theta_t}(x_t)$$

- The inverse can be recovered from fixed point iteration if Lip(g) < 1.

$$x_t^0 := x_{t+1}$$

$$x_t^{k+1} := x_{t+1} - g_{\theta_t}(x_t^k)$$



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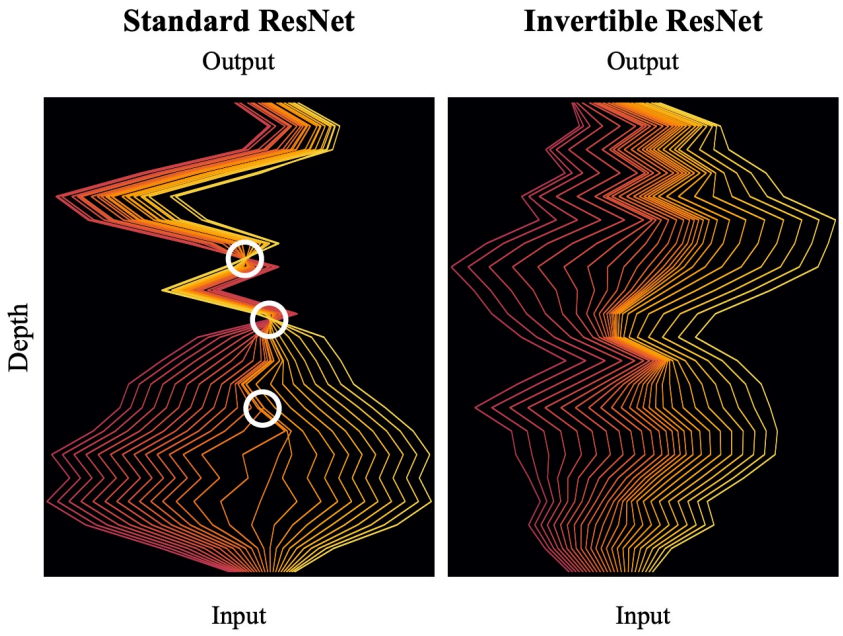
- MAF uses lower triangular Jacobian structure while iResNet uses approximation.



Behrmann et al. Invertible Residual Networks. ICML 2019.

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Estimating Jacobian Determinant

Grathwohl et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models. ICML 2019.
Behrmann et al. Invertible Residual Networks. ICML 2019.

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Estimating Jacobian Determinant

- Using power series to estimate det J.

$$\log|\det J_F| = \operatorname{tr}(\log J_F).$$

$$\operatorname{tr}(\log(I + J_g)) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{\operatorname{tr}(J_g^k)}{k}.$$

Grathwohl et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models. ICML 2019.
Behrmann et al. Invertible Residual Networks. ICML 2019.

Estimating Jacobian Determinant

- Using power series to estimate det J.

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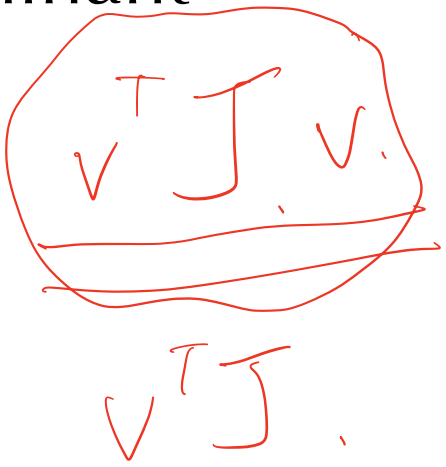

- To compute the trace without the full Jacobian. Use a stochastic estimate:

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Grathwohl et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models. ICML 2019.
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Draw v from $\mathcal{N}(0, I)$
$w^T := v^T$
$\ln\det := 0$
for $k = 1$ **to** n **do**
  $w^T := w^T J_g$ (vector-Jacobian product)
  $\ln\det := \ln\det + (-1)^{k+1} w^T v/k$
end for

Grathwohl et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models. ICML 2019.
Behrmann et al. Invertible Residual Networks. ICML 2019.

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Summary: Normalizing Flow

- Requires invertibility and tractability on Jacobian determinant
- Constraint on the functional form
- Or estimation of Jacobian / iterative inverse (numerical approximation).

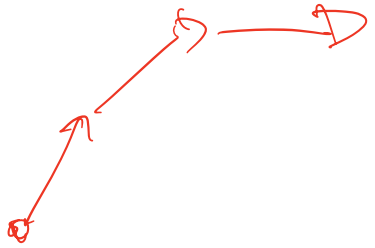
power series + stochastic estimate.

fixed.

Inference as Integration

- Residual Flow: $\phi(x) = x + \delta u(x)$

$$\frac{\phi(x) - x}{\delta} = u(x)$$



Inference as Integration

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CNF

- Can be written in continuous time (continuous normalizing flow).

$$x_t = \phi_t(x_0) = x_0 + \int_0^t \delta u_s(x_s)\, ds.$$

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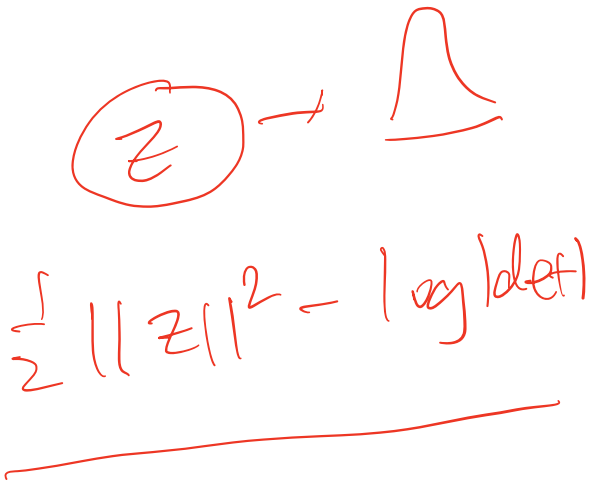
- Integration: Euler, or directly run an ODE solver
- Backprop solving an ODE without storing intermediate states

Flow Matching

- Taking integrals during training is cumbersome, and the learning signal from the top latent is weak.



Lipman et al. Flow Matching for Generative Modeling. ICLR 2023.

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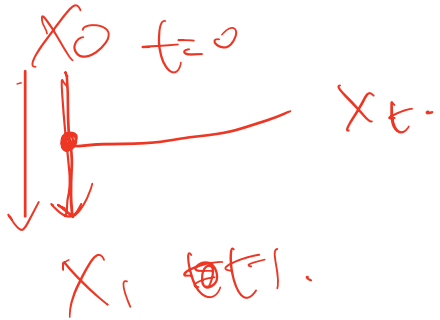
Flow Matching

- Taking integrals during training is cumbersome, and the learning signal from the top latent is weak.
- Given an original input x_1 and a noise x_0, $x_t = (1-t)x_0 + tx_1$



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- Want to fit a velocity $v_t(x)$ to match $u_t = x_1 - x_0$
- Flow Matching learning objective:

$$\mathcal{L}_{FM}(\theta) = \mathbb{E}_{t,x_0,x_1}[||v(x_t,t) - u_t(x_0,x_1)||^2]$$

Lipman et al. Flow Matching for Generative Modeling. ICLR 2023.

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Diffusion Models

- A popular generative model formulation.

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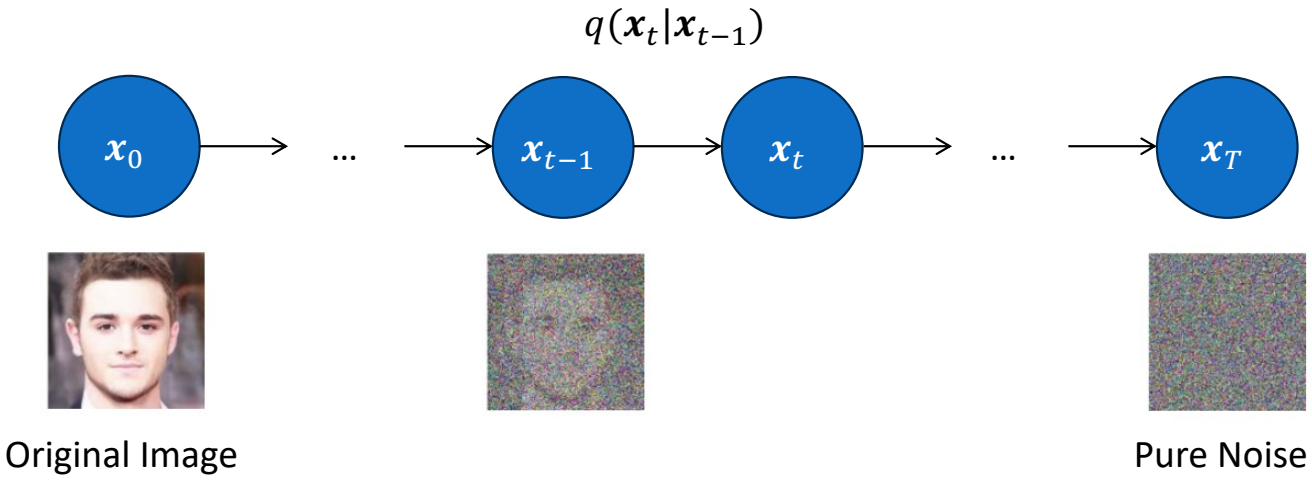
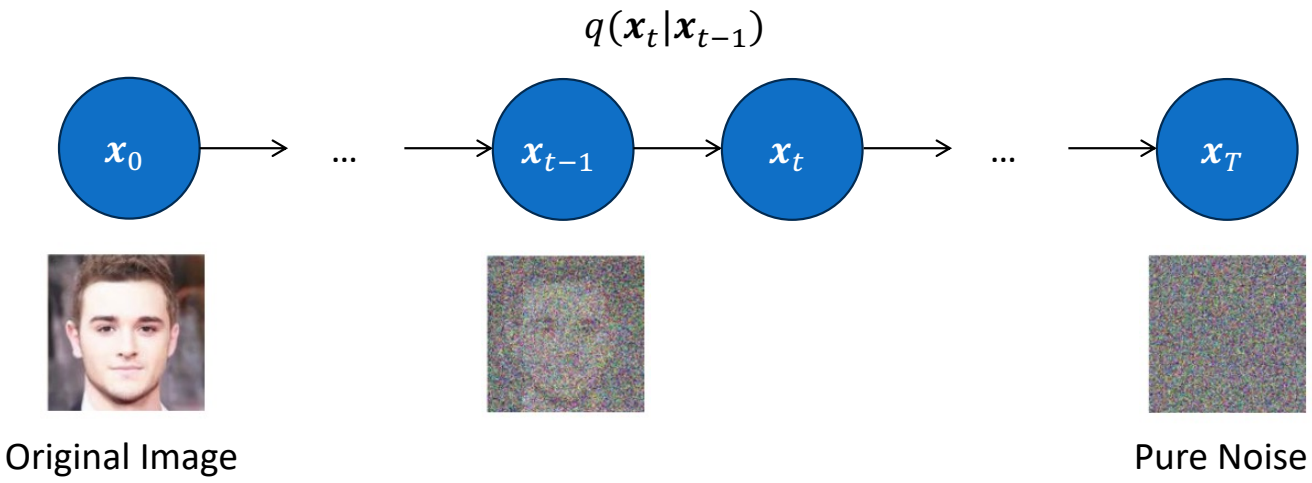


Diffusion Models

- Forward process: $q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$.



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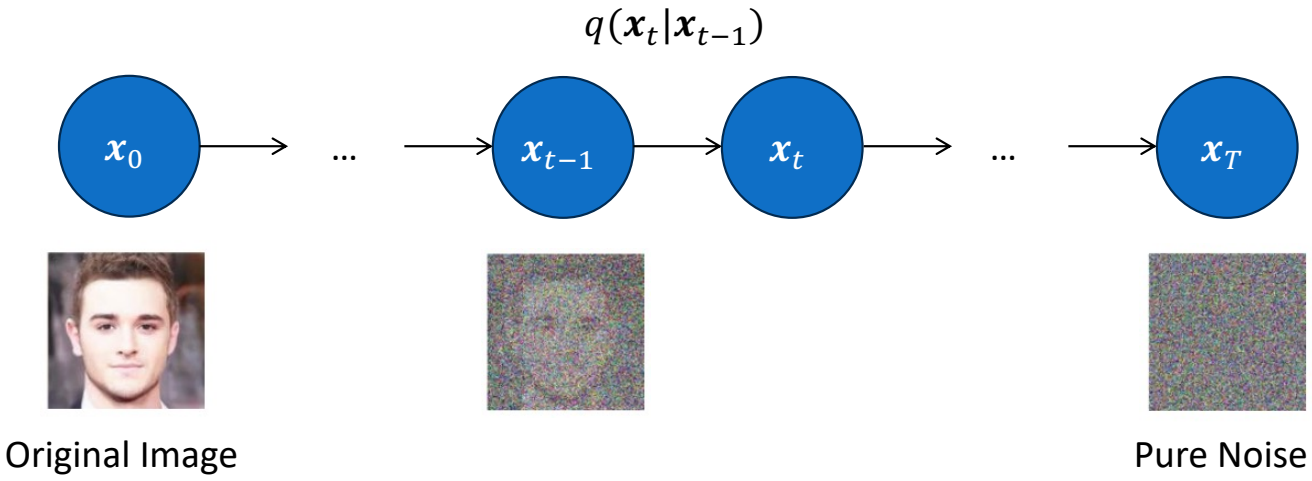
Diffusion Models

- Forward process: $q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$.
- You can also write: $x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_t,\ \epsilon_t \sim \mathcal{N}(0, I)$.



Properties of the Forward Process

- Forward process: $x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_t$

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Properties of the Forward Process

- Forward process: $x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_t$
- Write x_t as a function of x_0 with larger noises:

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)I).$$

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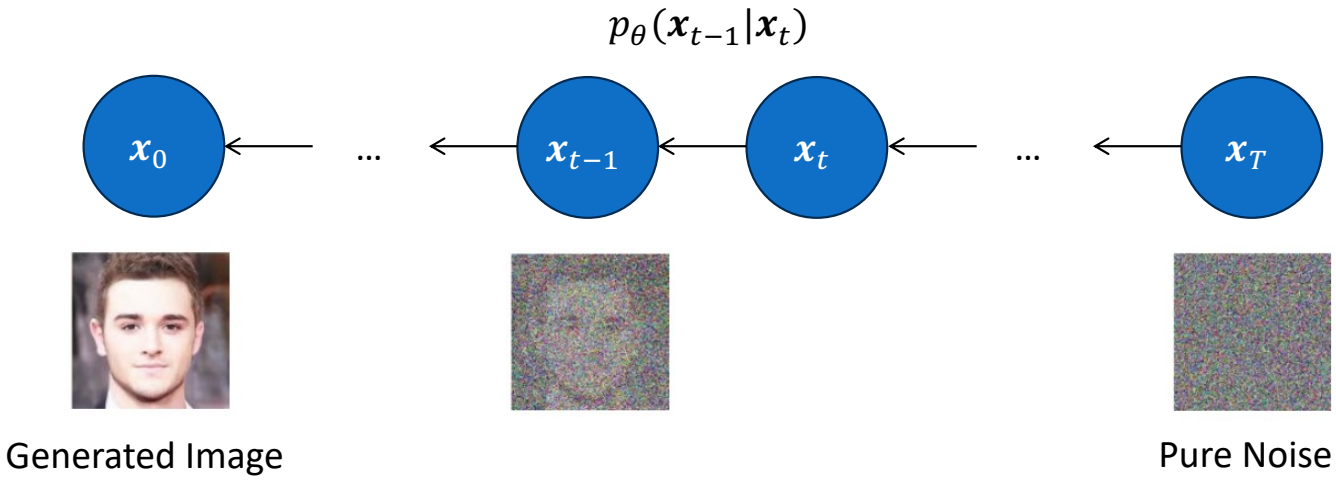
Reverse Process

- A generative model wants to predict x_0 from x_T.



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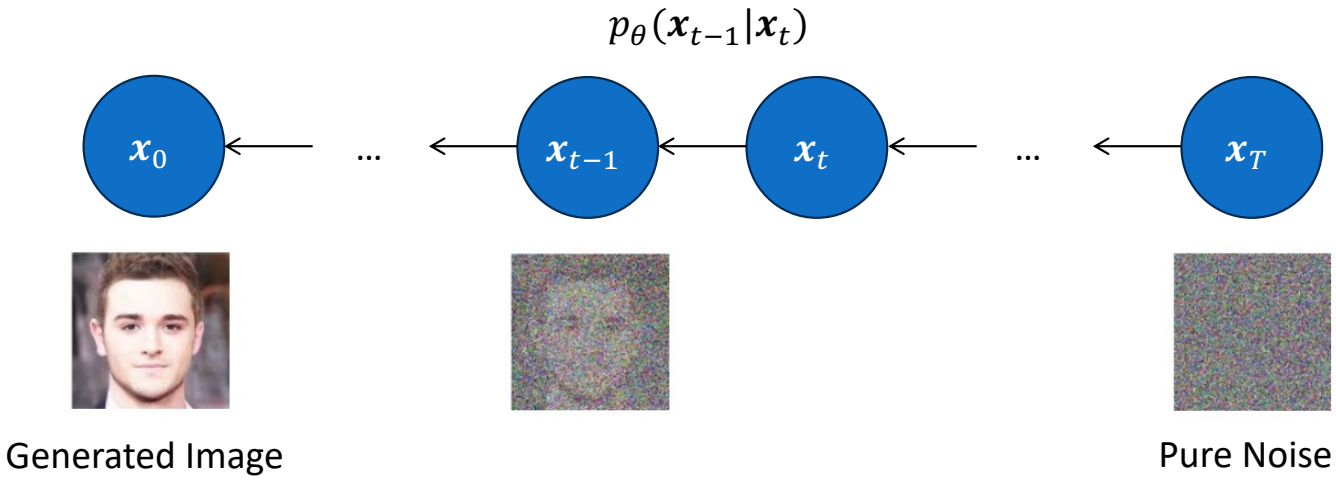
Reverse Process

- A generative model wants to predict x_0 from x_T.
- The reverse process transition is also Gaussian distributed. But we don't know what the transition will be like just by looking at the noisy image!



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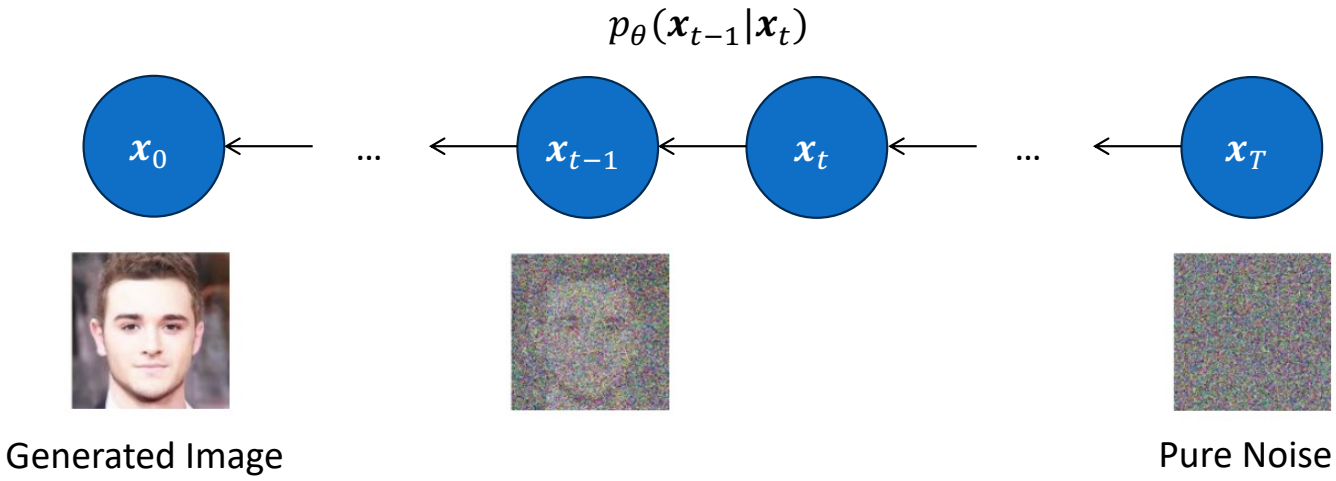
Reverse Process

- So, we need to learn a "model":

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t)).$$



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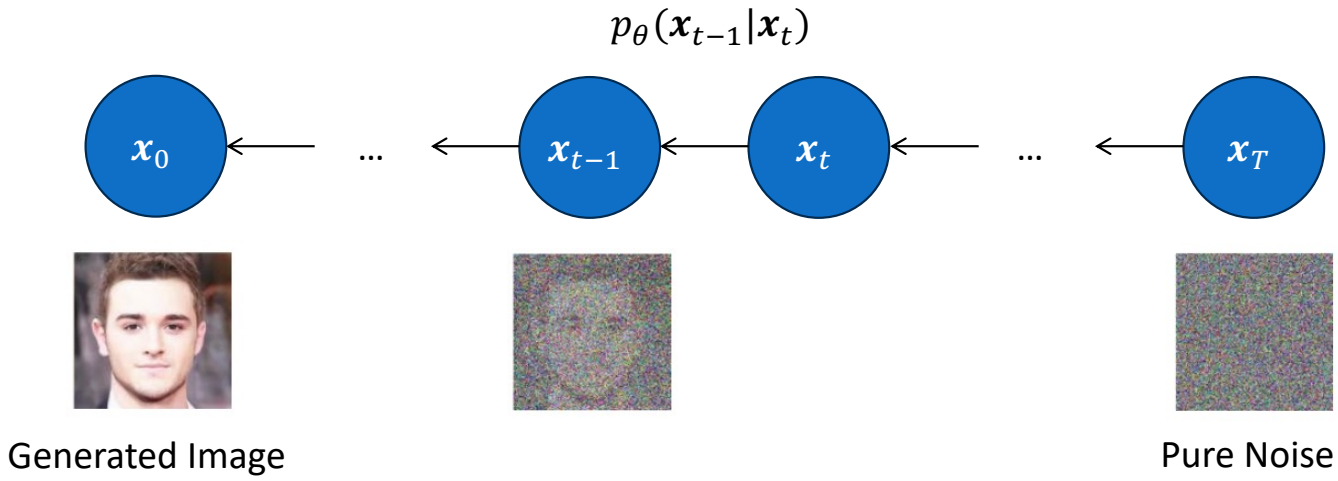
$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t)).$$

- μ_θ is the denoising vector.



Reverse Process

- Compute μ_θ? Derive $p(x_{t-1}|x_t)$.

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Reverse Process

- Compute μ_θ? Derive $p(x_{t-1}|x_t)$.
- Bayes rule:

$$q(x_{t-1}|x_t) = \frac{q(x_t|x_{t-1})q(x_{t-1})}{q(x_t)}.$$

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- Solution: Condition on the original input x_0:

$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1})q(x_{t-1}|x_0)}{q(x_t|x_0)}.$$

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Reverse Process

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Reverse Process

$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1})q(x_{t-1}|x_0)}{q(x_t|x_0)}.$$

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$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1})q(x_{t-1}|x_0)}{q(x_t|x_0)}.$$

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$$\tilde{\mu}_t = \frac{\sqrt{\alpha_t}\bar{\beta}_{t-1}}{\bar{\beta}_t} x_t + \frac{\sqrt{\alpha_{t-1}}\beta_t}{\bar{\beta}_t} x_0 = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon).$$

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- Want: train up a μ_θ to match with $\tilde{\mu}_t$.

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Training

- Sometimes it is more common to predict the denoising vector ϵ instead of μ.

$$\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon),$$

$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t)).$$

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- Sometimes it is more common to predict the denoising vector ϵ instead of μ.
- Randomly pick at a time step and predict the difference between the noisy and the original.

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Training

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- Randomly pick at a time step and predict the difference between the noisy and the original.

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
6: **until** converged

$$\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon),$$

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Sampling

- How do we sample an image?

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \dots, 1$ **do**
3: $\quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\quad \mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

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Sampling

- How do we sample an image?
- We know μ_θ which will help us transition from x_t to x_{t-1}.

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- Sample from $\mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma_t^2)$. σ_t can either be β_t or $\tilde{\beta}_t$ derived from the posterior.

Algorithm 2 Sampling

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2: **for** $t = T, \dots, 1$ **do**
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Deep Generative Models Summary

Guided Diffusion

- We can add guidance on the diffusion updates at inference time.

Classifier Guidance / External Score Model

$$x_{t-1} \leftarrow \text{sample from } \mathcal{N}(\mu + s\Sigma \nabla_{x_t} \log p_\phi(y|x_t), \Sigma)$$

$$\hat{\epsilon} \leftarrow \epsilon_\theta(x_t) - \sqrt{1-\bar{\alpha}_t}\, \nabla_{x_t} \log p_\phi(y|x_t)$$
$$x_{t-1} \leftarrow \sqrt{\bar{\alpha}_{t-1}} \left(\frac{x_t - \sqrt{1-\bar{\alpha}_t}\hat{\epsilon}}{\sqrt{\bar{\alpha}_t}} \right) + \sqrt{1-\bar{\alpha}_{t-1}}\hat{\epsilon}$$

Dhariwal & Nichol. Diffusion Models Beat GANs on Image Synthesis. NeurIPS 2021.
Ho & Salimans. Classifier-Free Diffusion Guidance. 2022.

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- We also can train a conditional diffusion model.

repeat
- $(\mathbf{x}, \mathbf{c}) \sim p(\mathbf{x}, \mathbf{c})$ ▷ Sample data with conditioning from the dataset
- $\mathbf{c} \leftarrow \varnothing$ with probability p_{uncond} ▷ Randomly discard conditioning to train unconditionally
- $\lambda \sim p(\lambda)$ ▷ Sample log SNR value
- $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- $\mathbf{z}_\lambda = \alpha_\lambda \mathbf{x} + \sigma_\lambda \boldsymbol{\epsilon}$ ▷ Corrupt data to the sampled log SNR value
- Take gradient step on $\nabla_\theta \left\| \boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c}) - \boldsymbol{\epsilon} \right\|^2$ ▷ Optimization of denoising model

until converged

Dhariwal & Nichol. Diffusion Models Beat GANs on Image Synthesis. NeurIPS 2021.
Ho & Salimans. Classifier-Free Diffusion Guidance. 2022.

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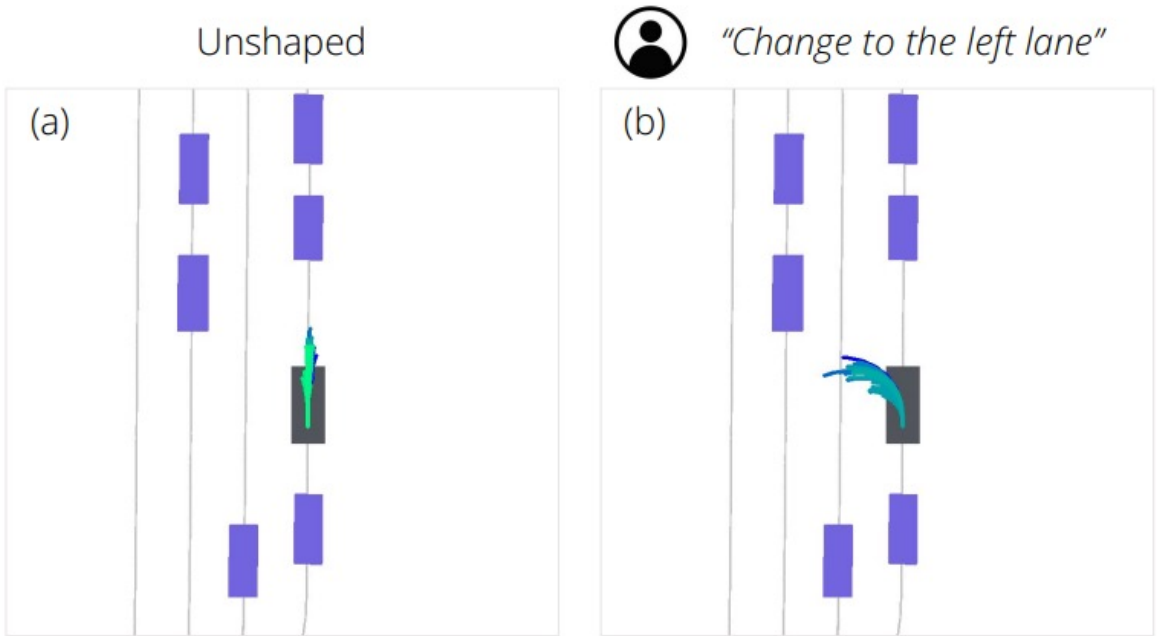
Test-Time Guidance / Adaptation

- Diffusion can be combined / guided at test time.



Yang et al. Diffusion-ES: Gradient-free Planning with Diffusion for Autonomous and Instruction-guided Driving. CVPR 2024.

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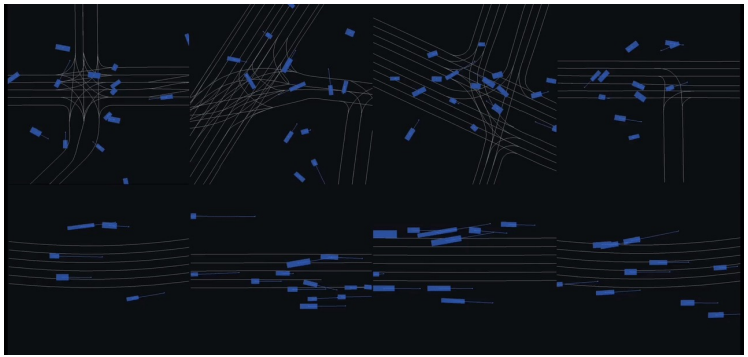
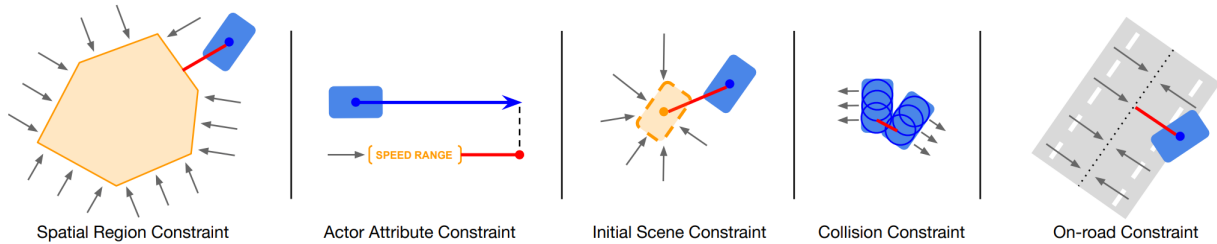
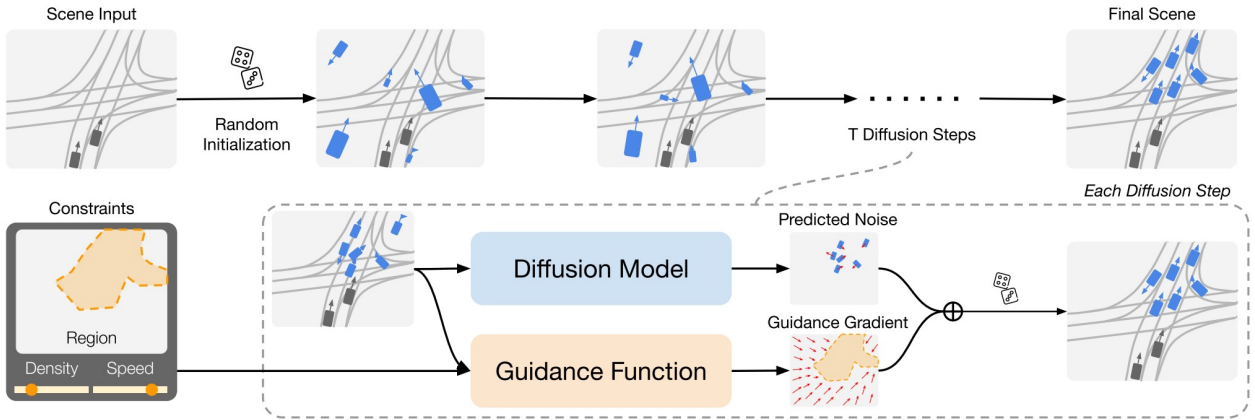
Generating Simulation Scenes







Lu et al. SceneControl: Diffusion for Controllable Traffic Scene Generation. ICRA 2024.

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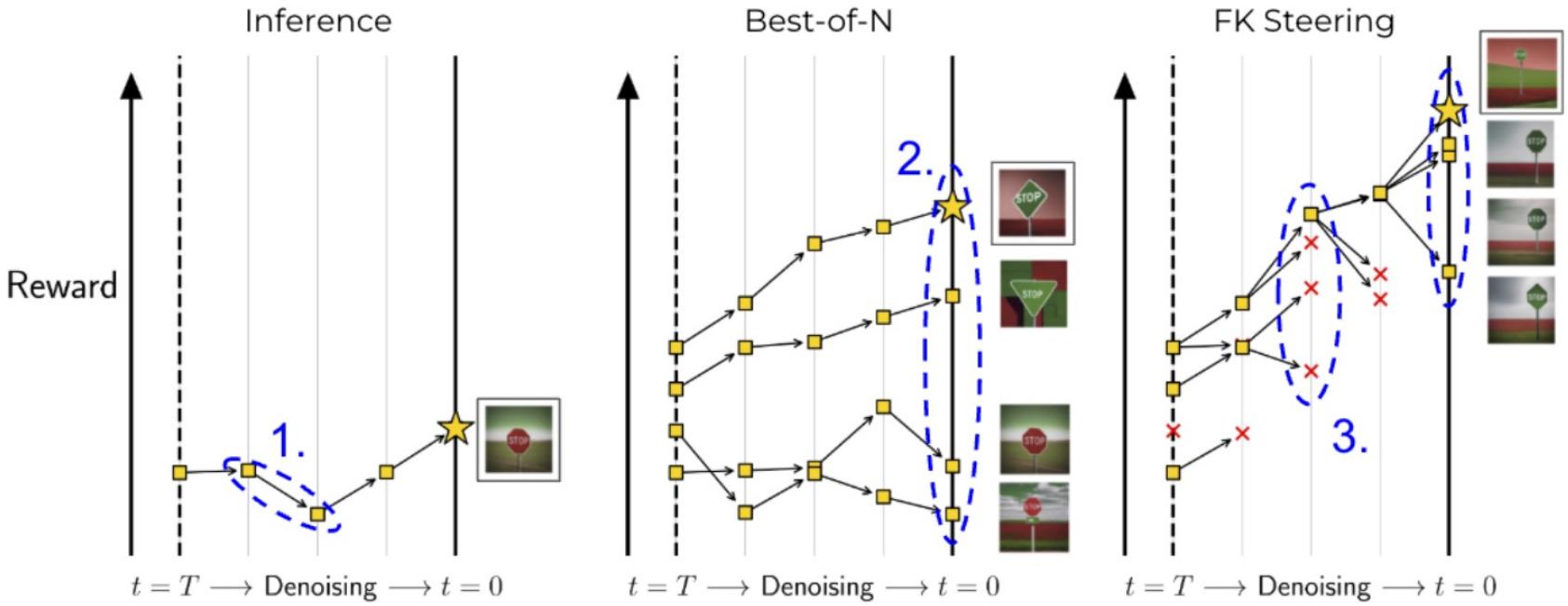
Non-Differentiable Rewards?



Prompt: *"a green stop sign in a red field"*

(1) Iteratively de-noise $x_T \rightarrow x_{T-1} \rightarrow \ldots \rightarrow x_0$.
(2) Generate multiple samples (*particles*).
(3) Resample promising particles at *intermediate* steps.

Singhal et al. A general framework for inference-time scaling and steering of diffusion models. ICML 2025.

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Diffusion Models for Detection

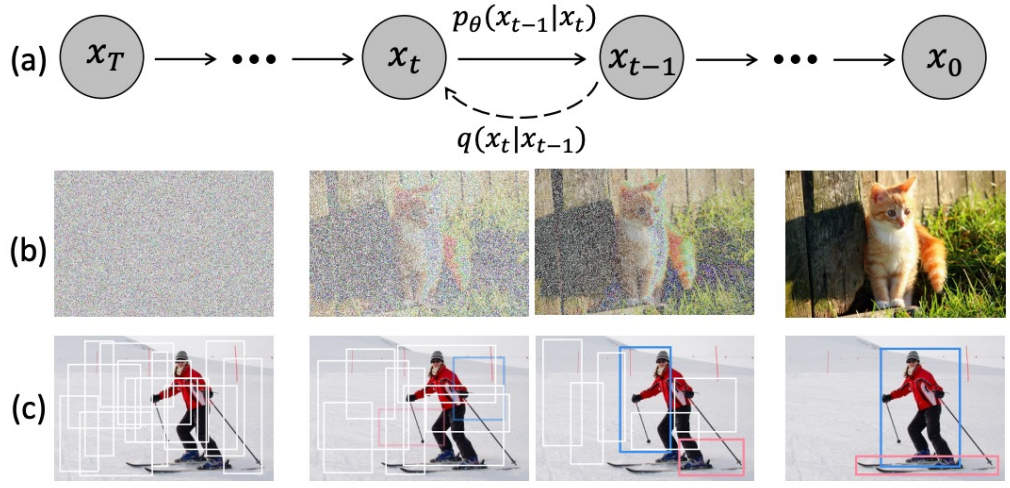
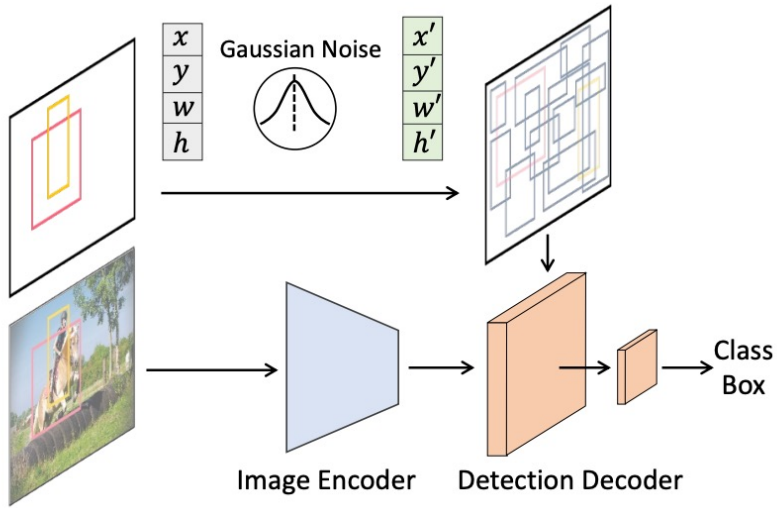


Figure 1. **Diffusion model for object detection**. (a) A diffusion model where q is the diffusion process and p_θ is the reverse process. (b) Diffusion model for image generation task. (c) We propose to formulate object detection as a denoising diffusion process from noisy boxes to object boxes.



Chen et al. DiffusionDet: Diffusion Model for Object Detection. ICCV 2023.

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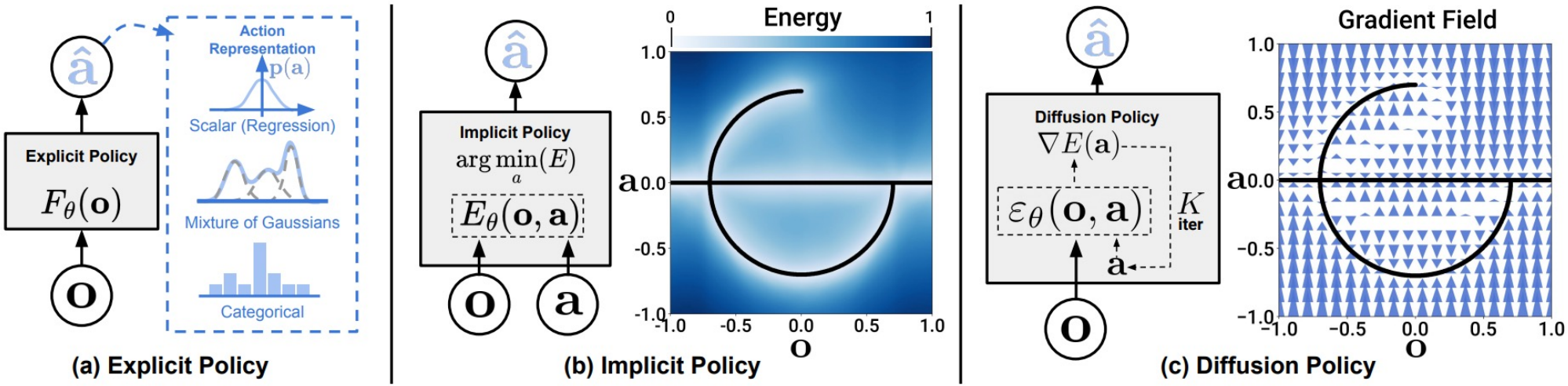
Planning and Control



Chi et al. Diffusion Policy: Visuomotor Policy Learning via Action Diffusion. RSS 2023.

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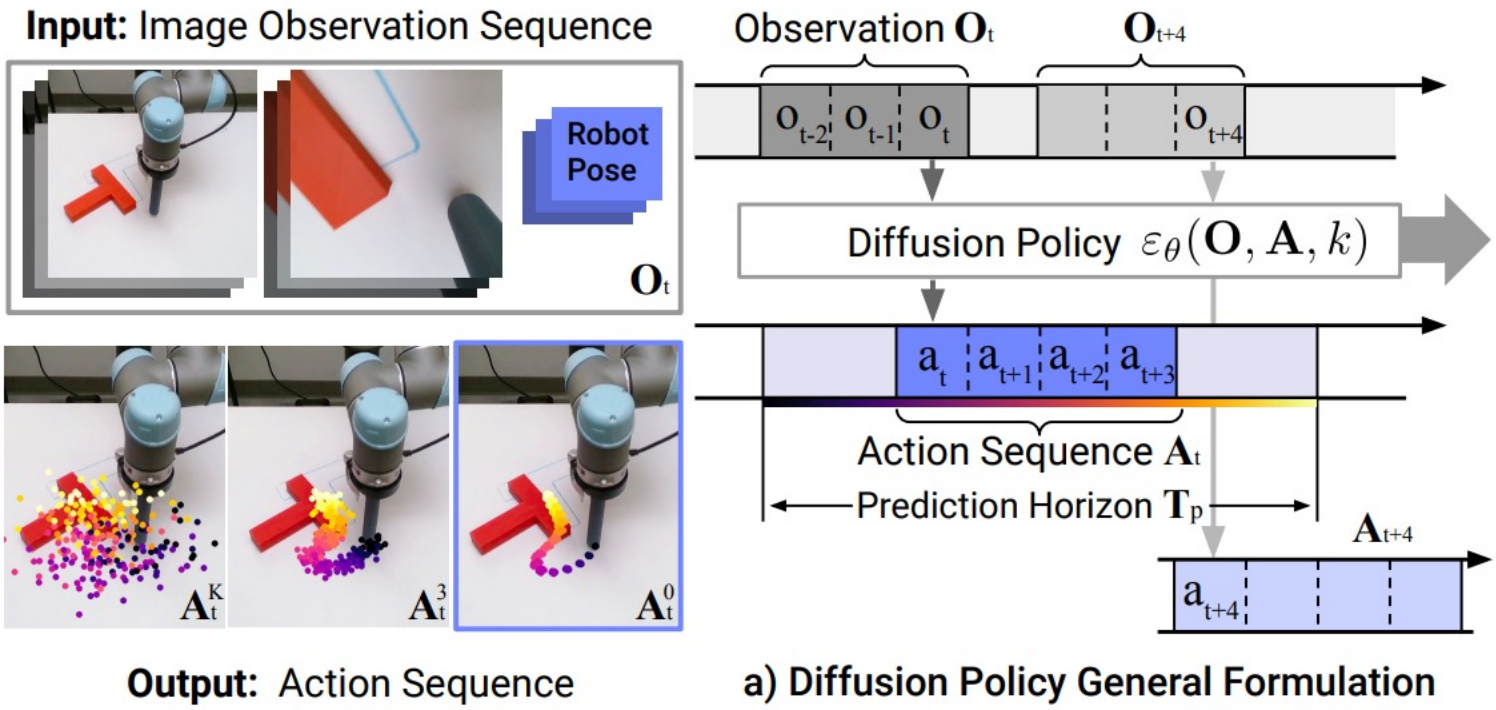
Diffusion for Planning and Control



Chi et al. Diffusion Policy: Visuomotor Policy Learning via Action Diffusion. RSS 2023.

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Summary: DL for Structured Outputs

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- Understand relations, pros and cons.
- Application in embodied environments.

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What's Next

- Tutorial on HPC
- Next week: 3D vision, mapping

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