Augmentation and Amortization for Generative Models

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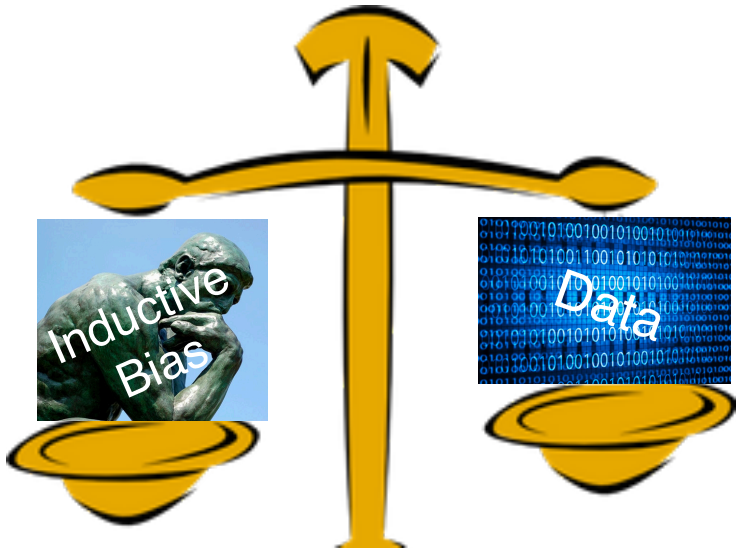
Inductive Bias versus Data

Generative models
(e.g. Bayesian networks)
+ lots of inductive bias
+ out of domain generalization

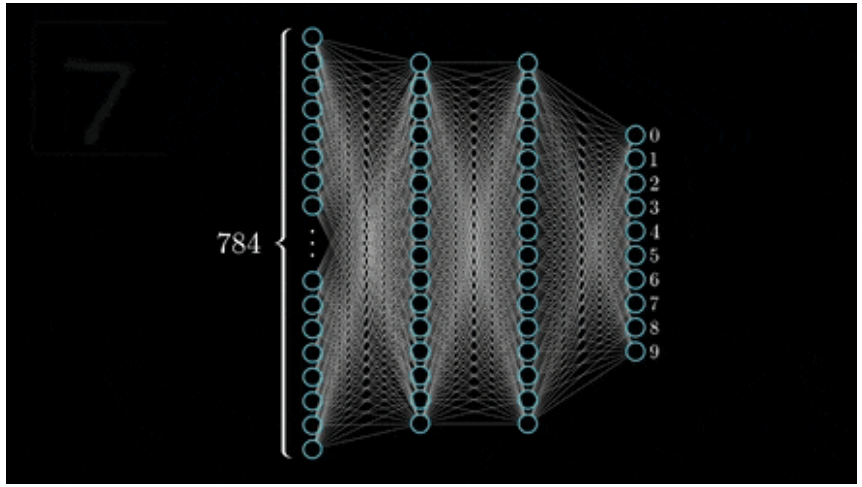
Inductive bias + data → predictions

Discriminative Models
(e.g. Deep learning)
+ lots of data
+ limited domain generalizatio



Discriminative Models

Raw data



Properties / class labels / semantic features

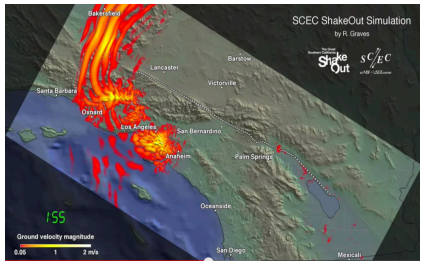
In ML we train discriminative models from raw data to class labels / system properties

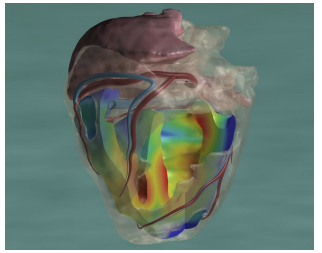
Generative / Forward Models

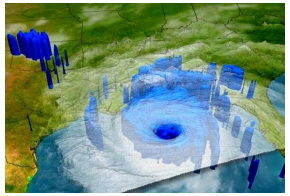
Definition: *A generative model simulates the data generation process.*

Examples:

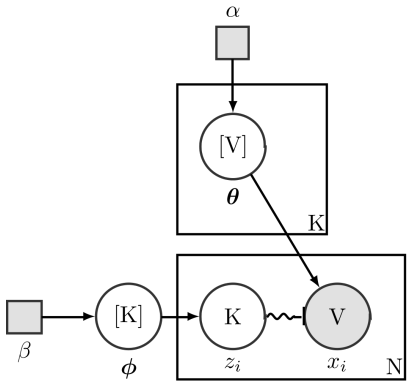
- Simulators
- Graphical models
- Probabilistic programs
- Ordinary/Partial differential equations

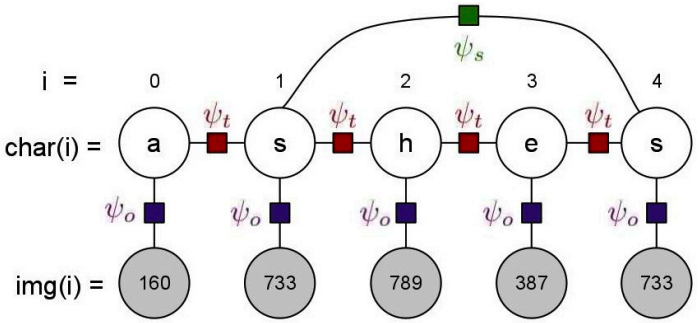


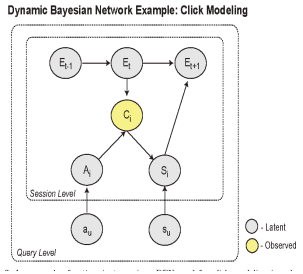




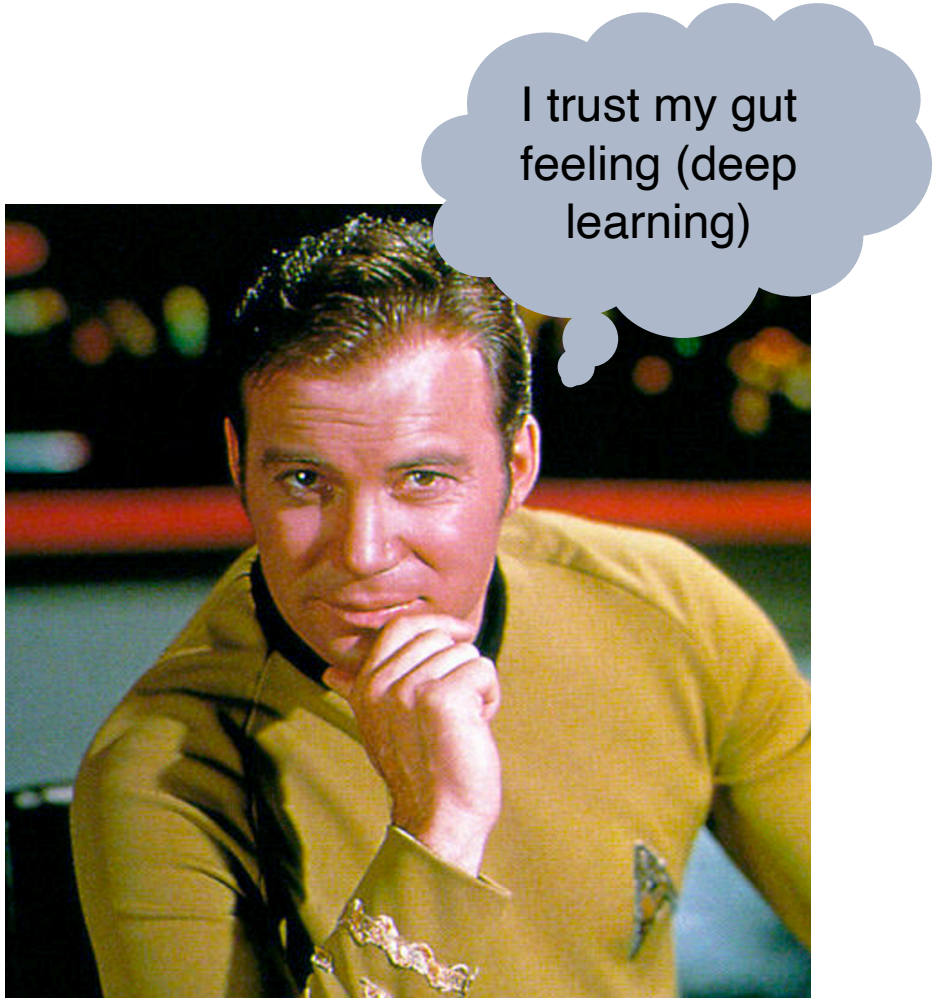
Also known as **forward models**



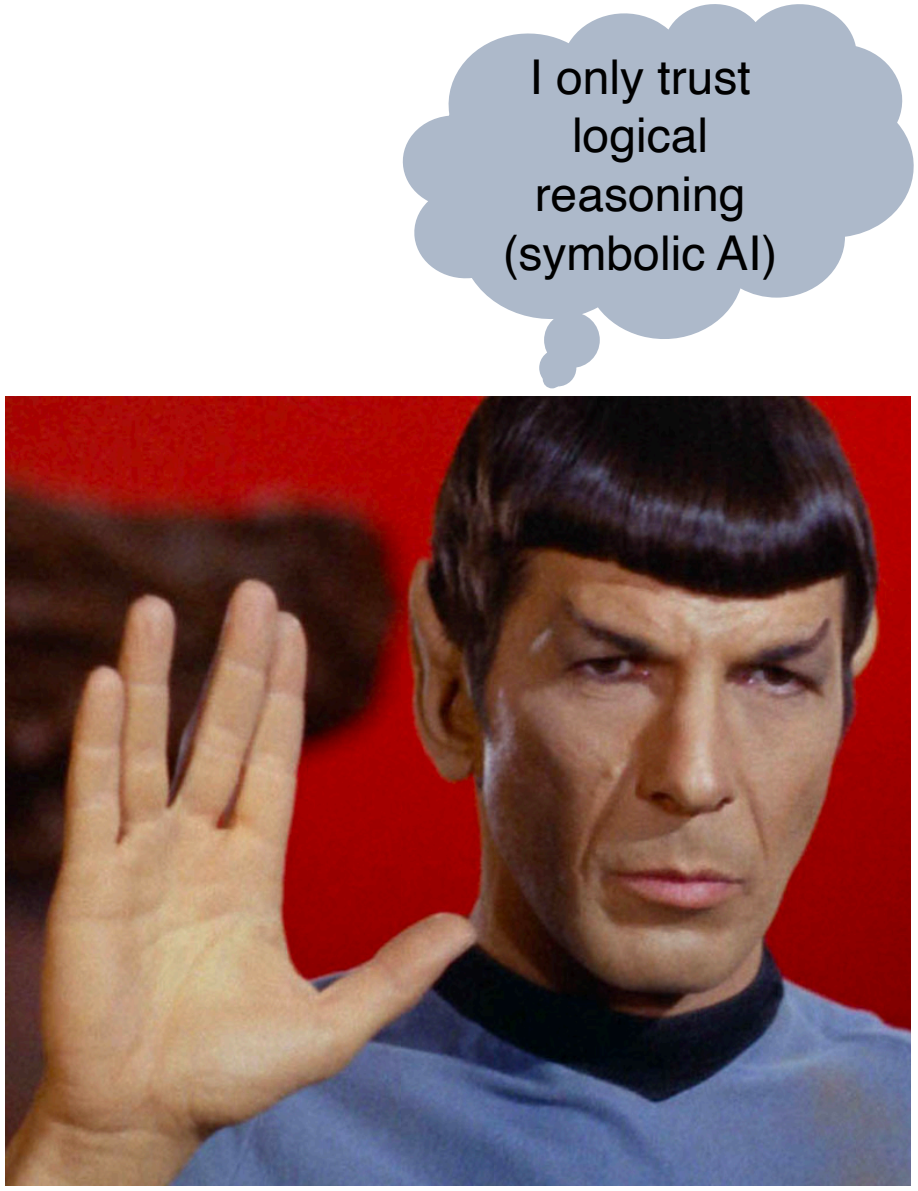




Intuition versus Logic

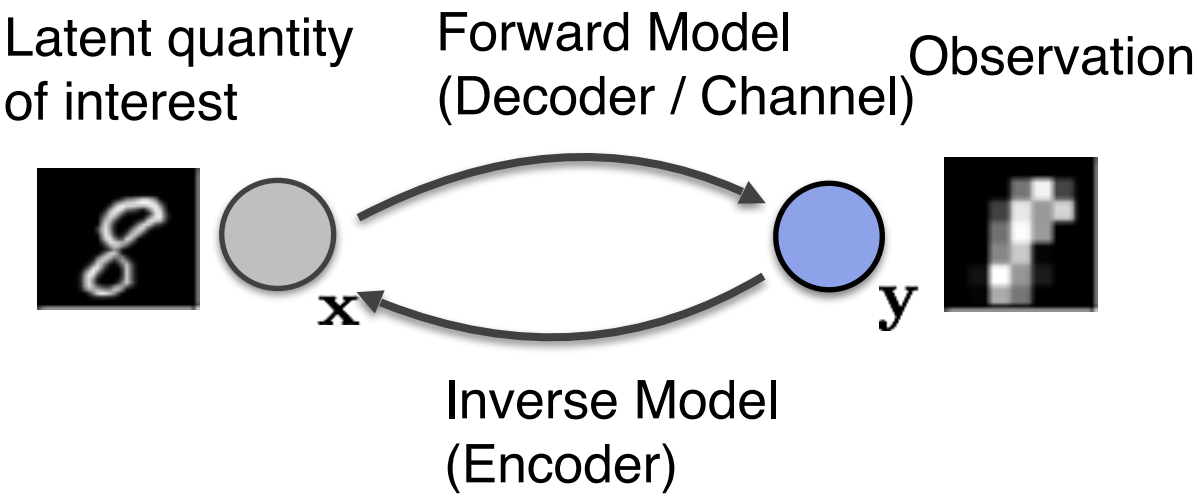


Kirk

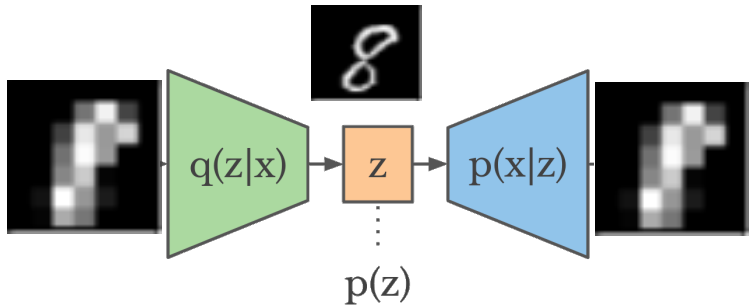


Spock

Forward Decoder & Inverse Encoder Models



VAE: Variational Autoencoder



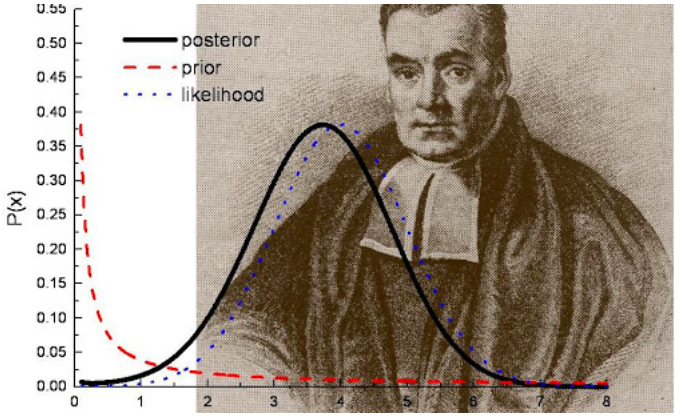
$$y = g(x) + \epsilon$$

$$\hat{x} = h(y)$$

Forward (Decoder) Model $y \sim p(y|x)$

Inverse (Encoder) Model $\hat{x} \sim q(x|y)$

How are they related?



Thomas Bayes

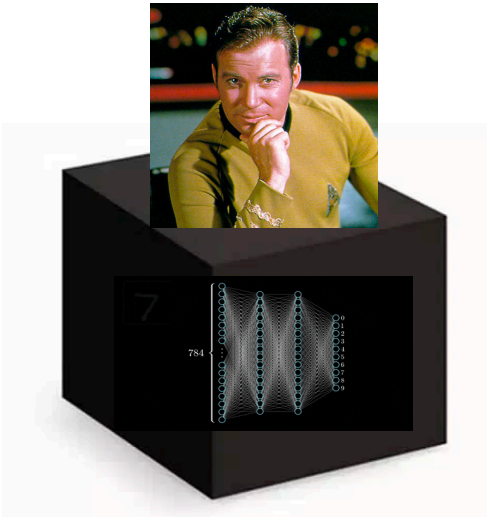
Bayes Rule:

Inverse model / Encoder

Forward model / Decoder

$$P_{discr}(\text{class}|\text{data}) = \frac{P_{gen}(\text{data}|\text{class})P_{prior}(\text{class})}{P(\text{data})}$$

Pros and Cons



White Box:

- **Data efficient**: model uses expert knowledge (e.g. laws of physics)
- **Interpretable**: variables mean something in the real world
- **Better generalization**: model uses causal structure

Black Box:

- **More flexible**: less biased to human imagination
- **Accurate**: you model your predictions directly
- **Fast** predictions: you don't need Bayes rule

We want to combine these strengths into one modeling paradigm

Amortization & Augmentation

Amortization

"Finding or generating related problems to learn a model or policy to do X"

- *Learning to Infer (VAE encoder)*: Instead of performing inference per instance (e.g. MF) learn a model to predict the outcome of inference.
- *Learning to optimize*: Instead of running a classical optimization tool (e.g. GA) learn a policy on similar optimization problems to build a better optimizer.
- *Learning to Learn (Meta-Learning):* Instead of learning a model using e.g. gradient descend, train an optimizer on related learning problems.

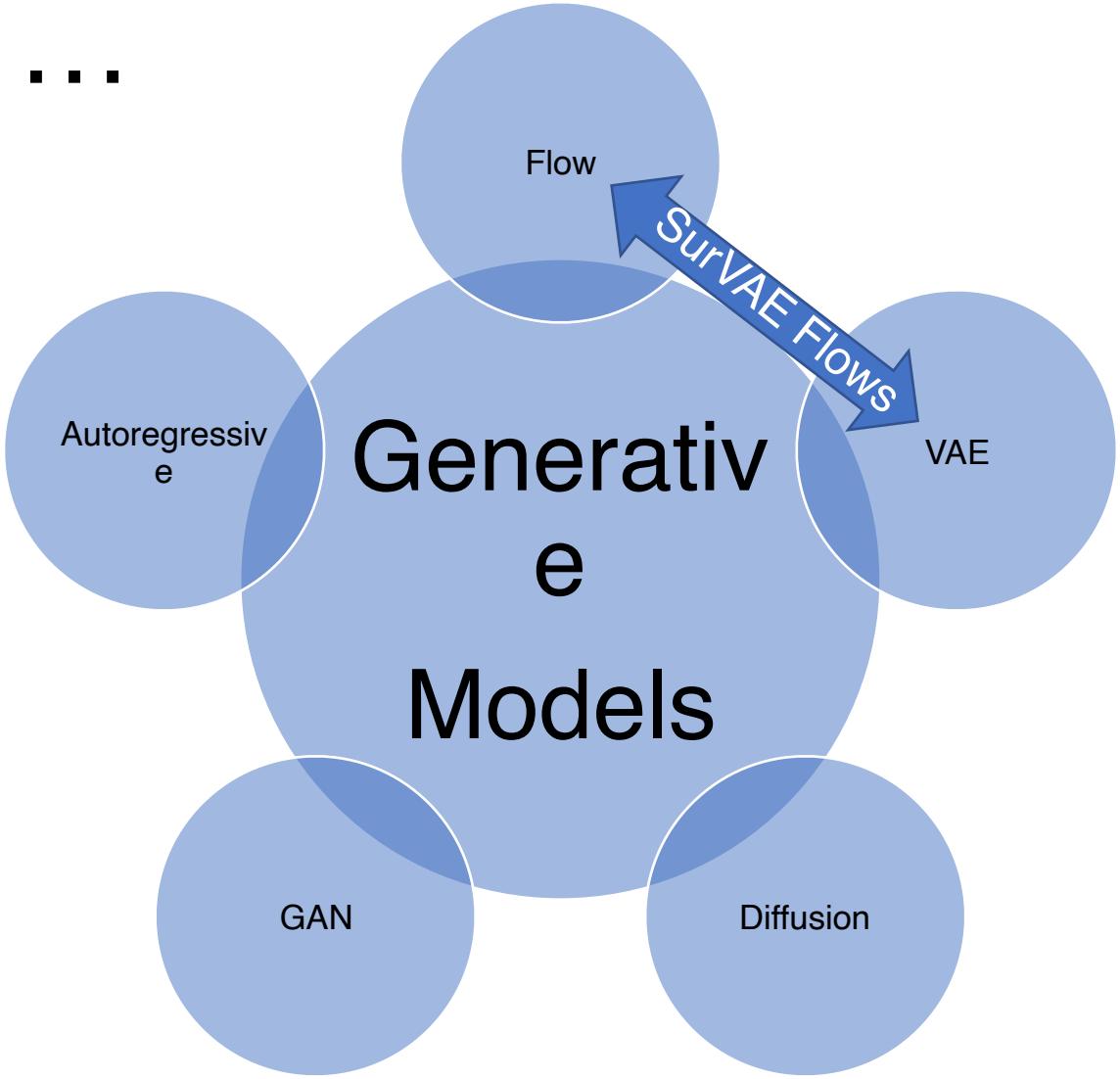
Augmentation

"A Hybrid system that combines classical, hand-engineered methods with learned ML-based models or policies"

- Probabilistic programs / simulators + neural networl
- Data forcing terms in encoders.
- Hybrid inference that combines classical inference in graphical models (e.g. BP, MF) with neural netwo (e.g. graph NN)s

Flows, GANs, VAEs, …

The state of world in terms of generative modeling



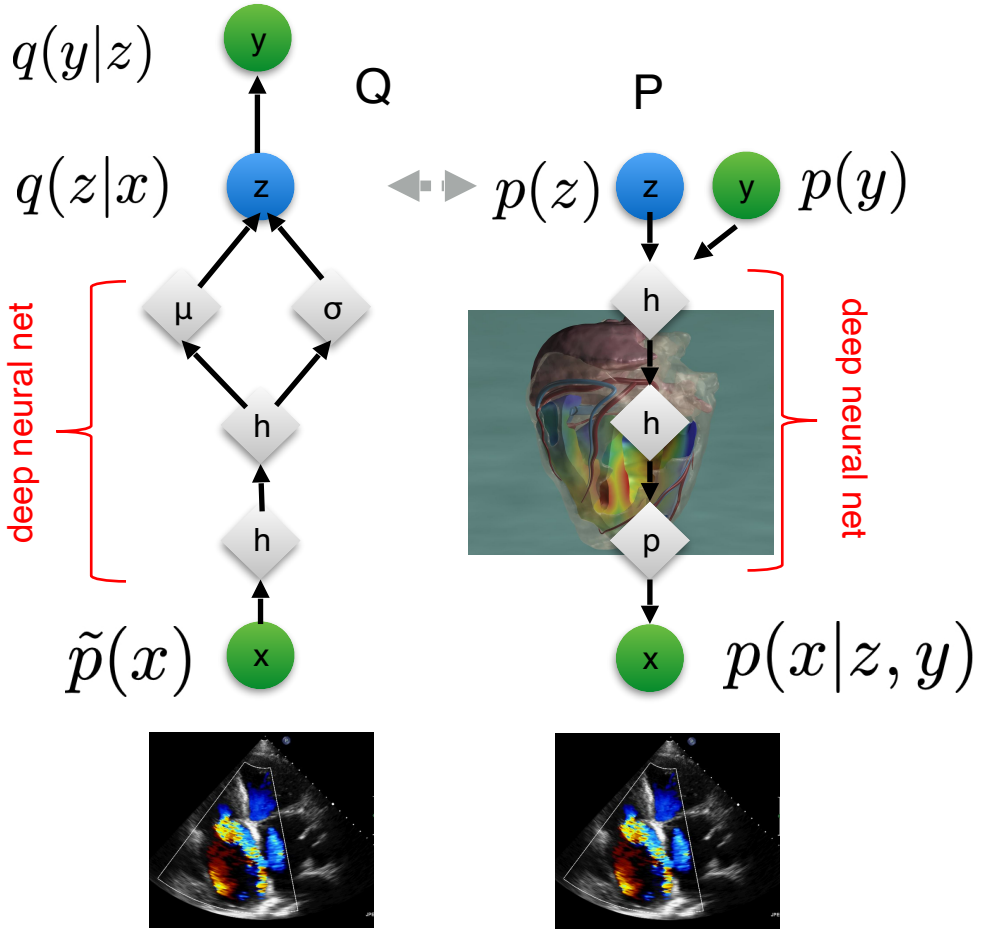
The Variational Auto-Encoder as Approximate Bayes Rule

(Kingma & W. 2014, Rezende et al, 2014)

deterministic NN node

unobserved stochastic node

observed stochastic node



Amortized encoder Augmented Decoder

VAE objective-function = ELBO:

$$\min_{\phi,\theta} KL[Q_\phi(Z|X)\hat{P}(X)||P(Z)P_\theta(X|Z)]$$

$$\min_{\phi,\theta} KL[\hat{P}(X)||P(X)] + E_{\hat{P}(X)}KL[Q(Z|X)||P(Z|X)]$$

$$\Rightarrow P(X) = \hat{P}(X) \quad \& \quad Q_\phi(Z|X) = \frac{P(Z)P_\theta(X|Z)}{P(X)}$$

Normalizing Flows Rezende & Mohamed 2015

- Deterministic (invertible) reparameterization of P(X):

$$\log P(X) = \log P(Z) + \log \left| \det \left(\frac{dZ(X)}{dX} \right) \right|$$

- Sequence of invertible transformations:

$$\log P(X = Z_T) = \log P(Z_0) + \sum_{t=1}^{T} \log \left| \det \left(\frac{dZ_t}{dZ_{t-1}} \right) \right|$$

Composable Transformations

- Normalizing flow: deterministic invertible transformation f:X→Z,

$$\log P(X) = \log P(Z) + \log \left| \det \left(\frac{dZ(X)}{dX} \right) \right|$$

- ELBO: Bound on stochastic transformation Q(Z|X),

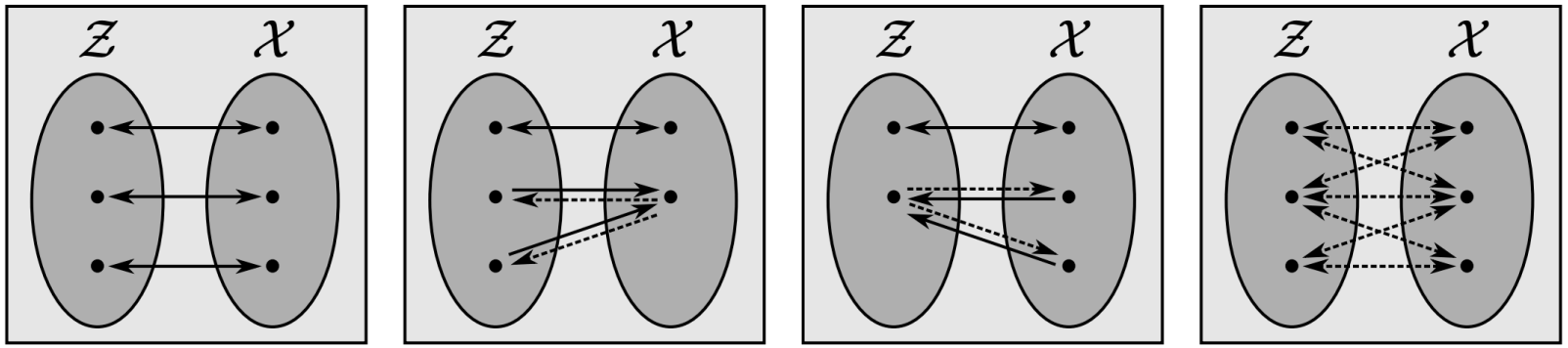
$$\log P(X) \geq E_Q \left[\log P(Z) \right] + E_Q \left[\log \left(\frac{P(X|Z)}{Q(Z|X)} \right) \right]$$

Algorithm 1: $\log - \text{likelihood}(\boldsymbol{x})$

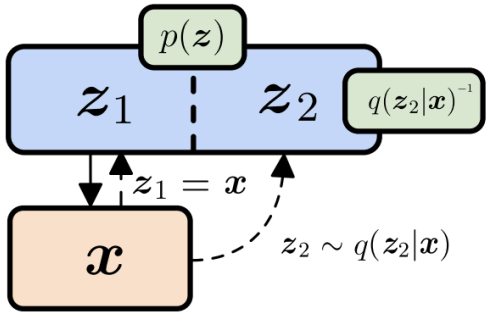
Data: $\boldsymbol{x}$, $p(\boldsymbol{z})$ & $\{f_t\}_{t=1}^{T}$
Result: $\mathcal{L}(\boldsymbol{x})$
for t *in* $\text{range}(T)$, **do**
  if f_t *is bijective* **then**
    $\boldsymbol{z} = f_t^{-1}(\boldsymbol{x})$;
    $\mathcal{V}_t = \log \left| \det \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} \right|$;
  else if f_t *is stochastic* **then**
    $\boldsymbol{z} \sim q_t(\boldsymbol{z}|\boldsymbol{x})$;
    $\mathcal{V}_t = \log \frac{p_t(\boldsymbol{x}|\boldsymbol{z})}{q_t(\boldsymbol{z}|\boldsymbol{x})}$;
  $\boldsymbol{x} = \boldsymbol{z}$;
end
return $\log p(\boldsymbol{z}) + \sum_{t=1}^{T} \mathcal{V}_t$

Surjections & SurVAE Flows

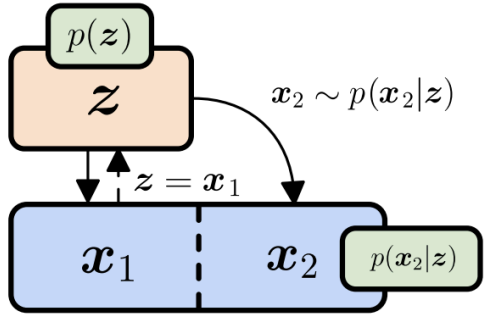
(Didrik Nielsen et al 2020)



(a) Bijective (b) Surjective (Gen.) (c) Surjective (Inf.) (d) Stochastic



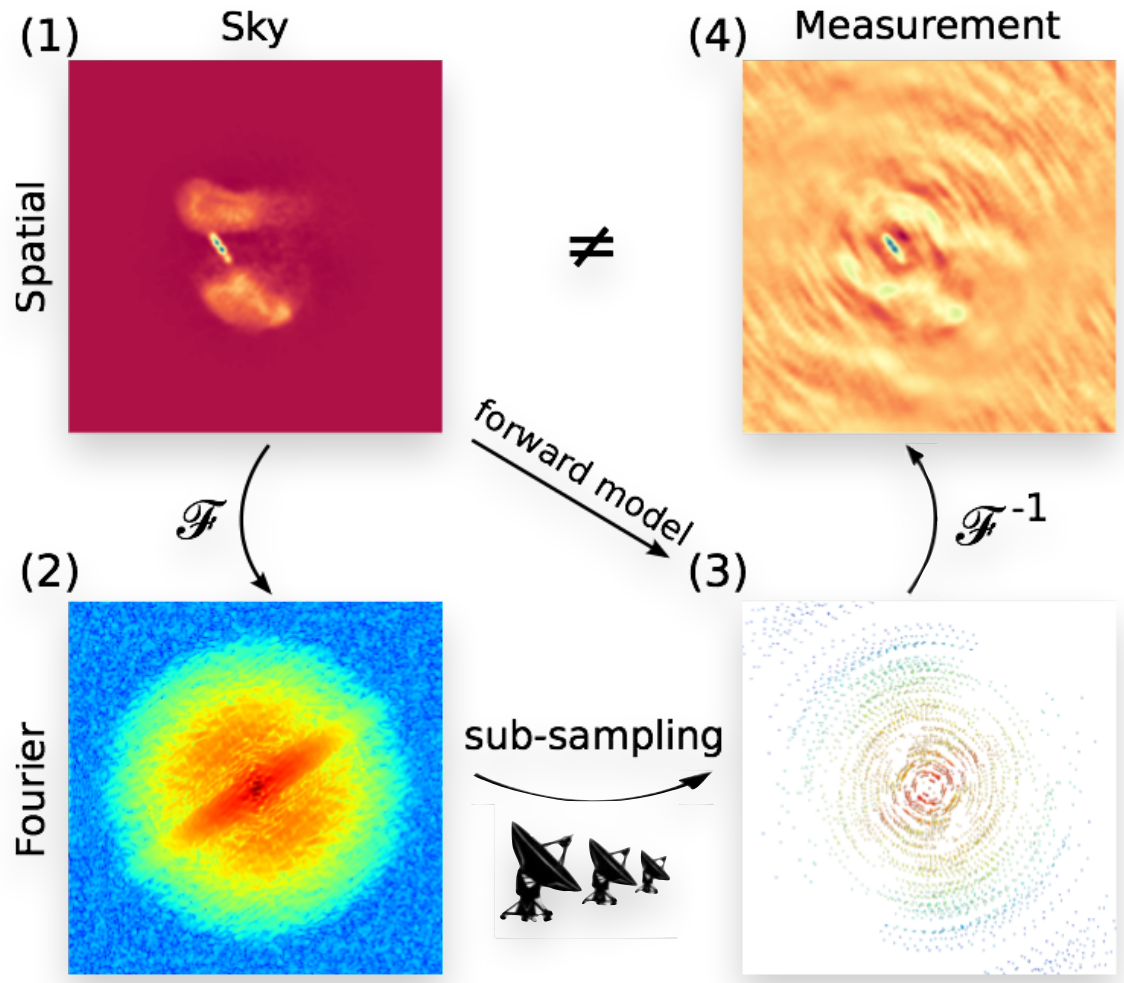
(a) Gen. slicing



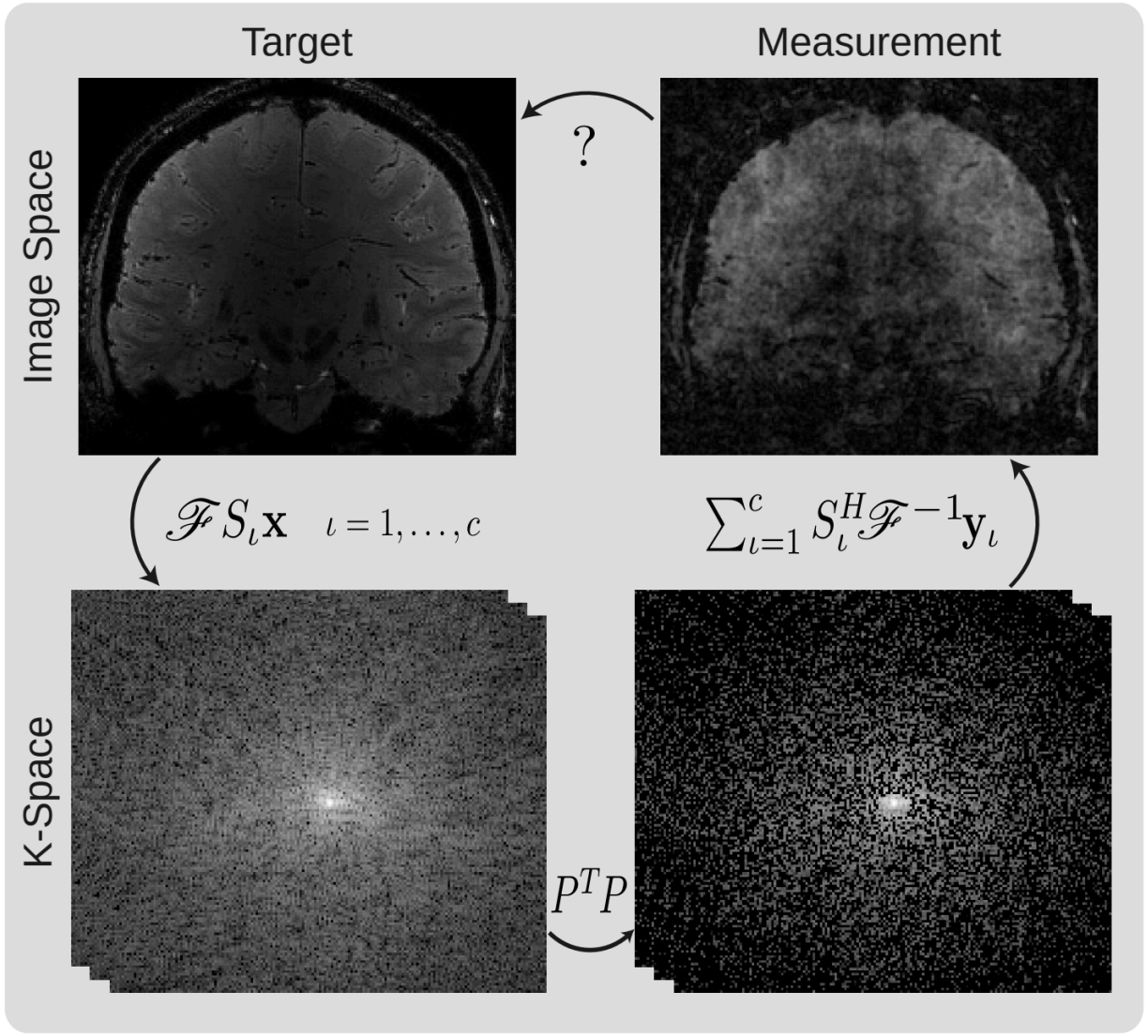
(b) Inf. slicing

ELLIS exchange

Inverse Problems: Radio Astronomy



Inverse Problems: MRI Reconstruction

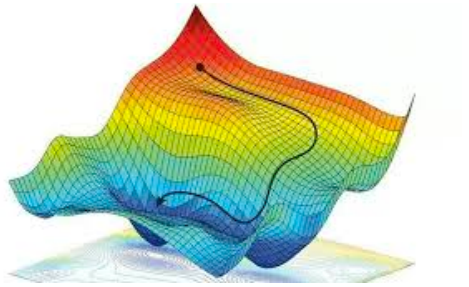


Classical Solutions

We will add neural components to a classical iterative optimization scheme

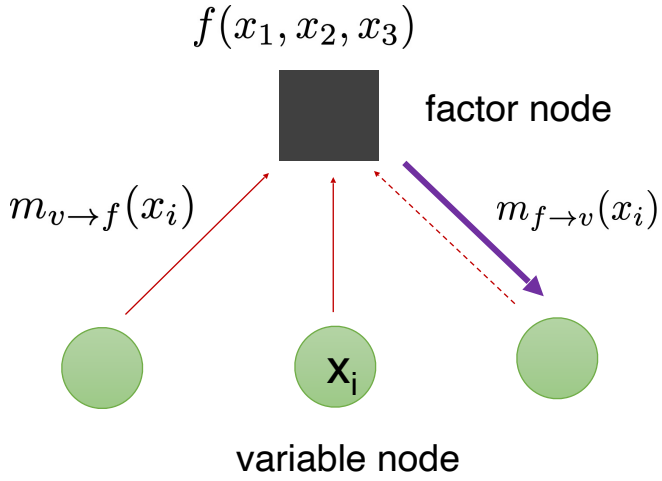
- Gradient ascent on objective $L(x) = \underbrace{\log P(y|x)}_{\text{observation model}} + \underbrace{\log P(x)}_{\text{learned prior}}$

$$x_{t+1} = x_t + \nabla_x L(x)|_{x=x_t}$$



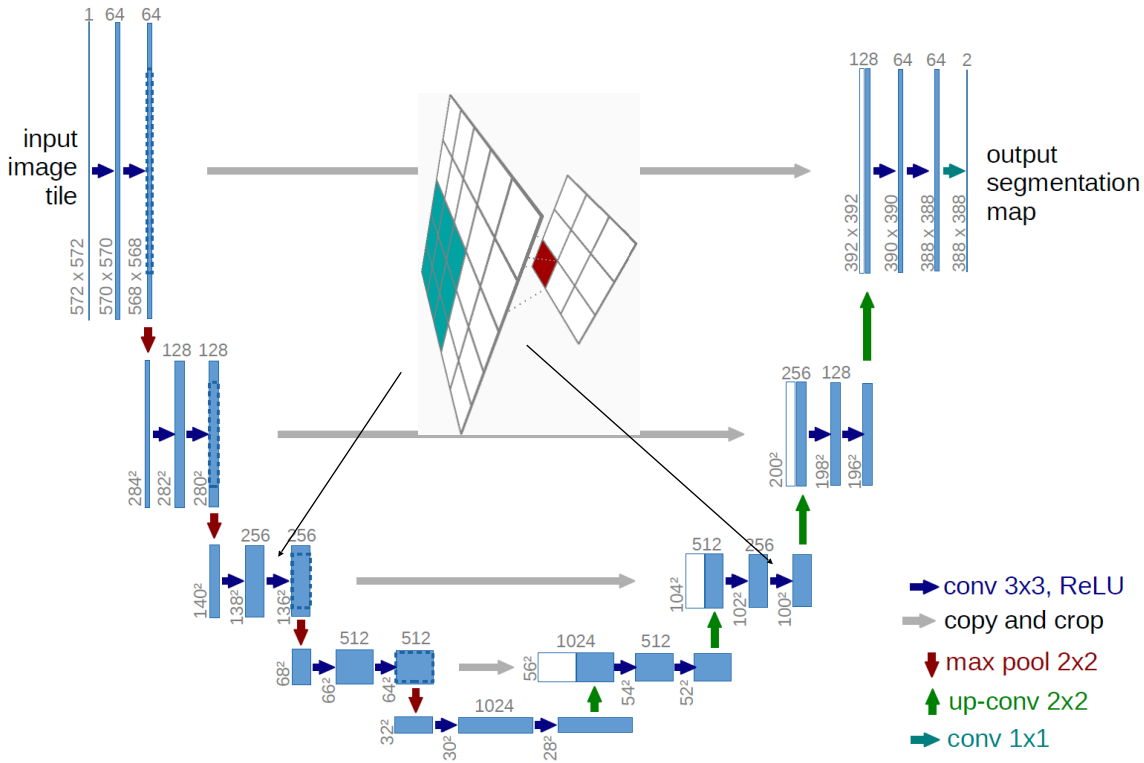
- Belief propagation or other inference algorithm

$$\mu_{f_s \to x_n}(x_n) = \sum_{\mathbf{x}_s \setminus x_n} f_s(\mathbf{x}_s) \prod_{m \in \mathcal{N}(f_s) \setminus n} \mu_{x_m \to f_s}(x_m)$$



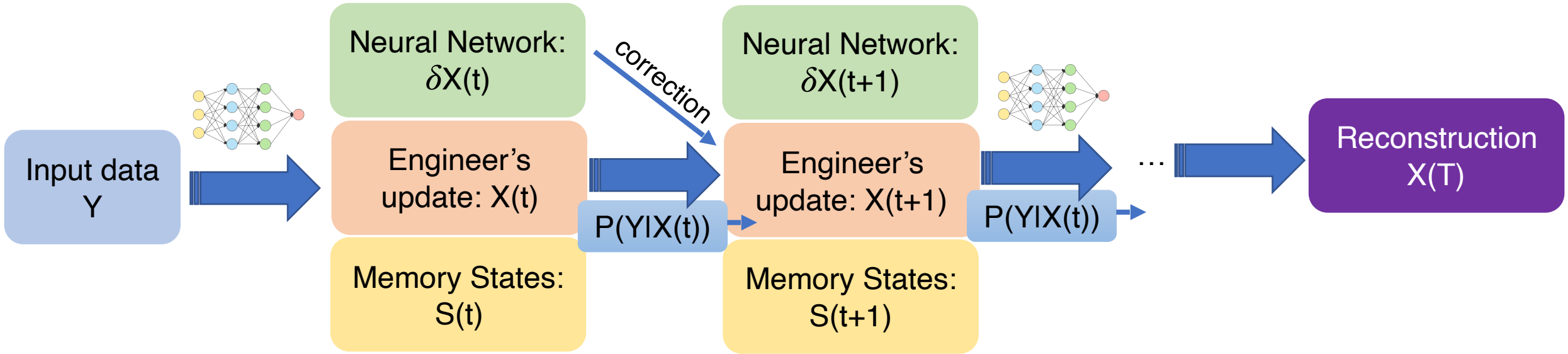
Deep Learning (Full Neural) Solution

- Obtain data pairs: $\{x_n, y_n\},\ n = 1..N$
- Train big neural net $X = f_\theta(Y)$



Amortized, Augmented Inverse (Encoder) Model

- Unroll classical iterative optimization scheme and interpret as RNN
- Add memory states S
- Train deep neural network to *correct* iterative engineering solution (neural augmentation)
- Use forward model P(Y|X) to check if current estimate agrees with data

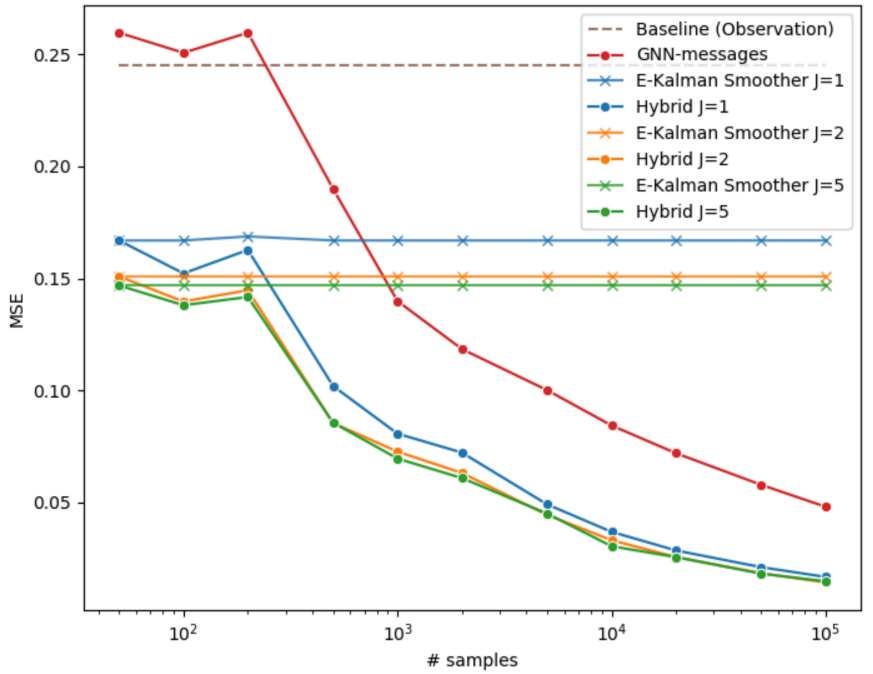


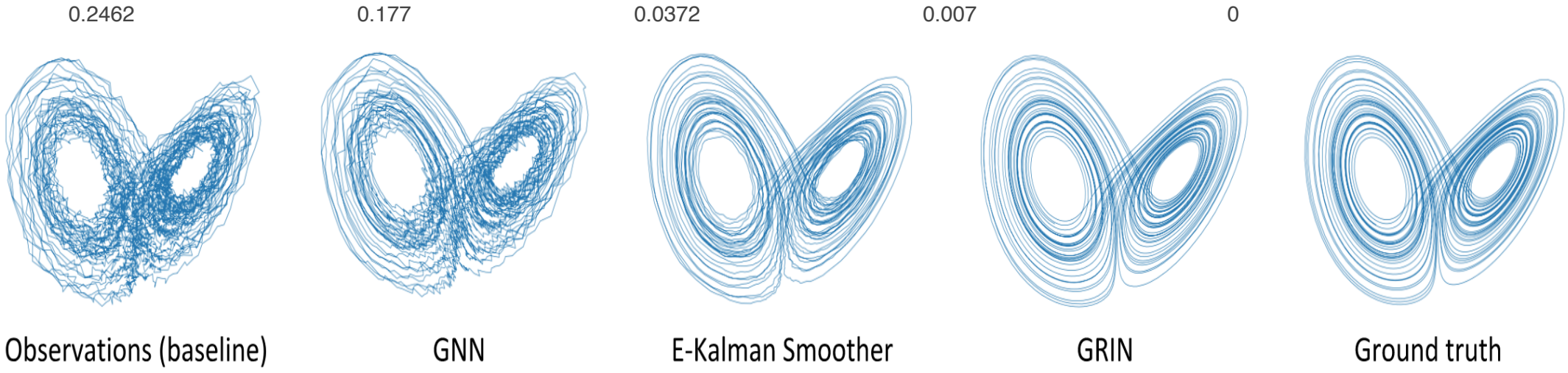
Nonlinear Kalman Filter

(Garcia et al 2019)

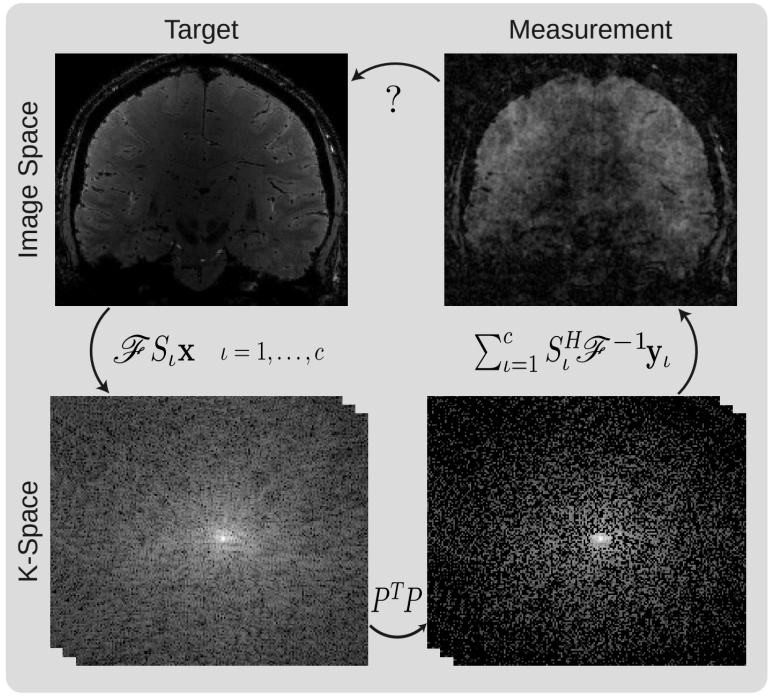
- Lorenz attractor dynamics (chaotic)

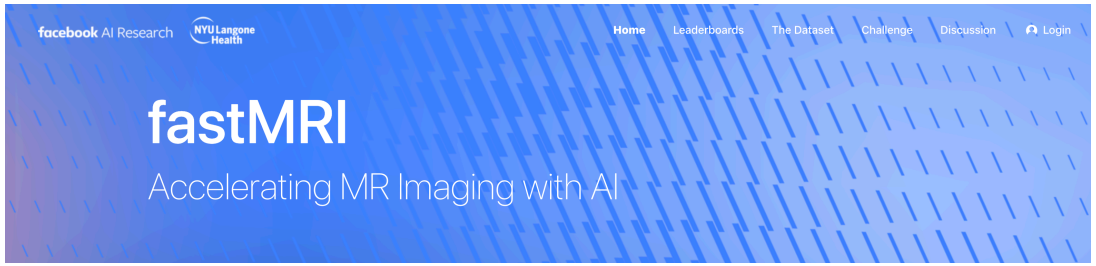
$$\frac{\partial z_1}{\partial t} = 10(z_2 - z_1)$$
$$\frac{\partial z_2}{\partial t} = z_1(28 - z_3) - z_2$$
$$\frac{\partial z_3}{\partial t} = z_1 z_2 - \frac{8}{3} z_3$$



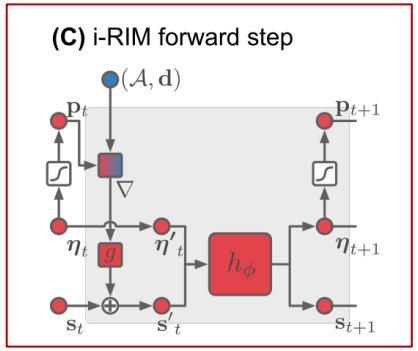


Example Problems: MRI Reconstruction

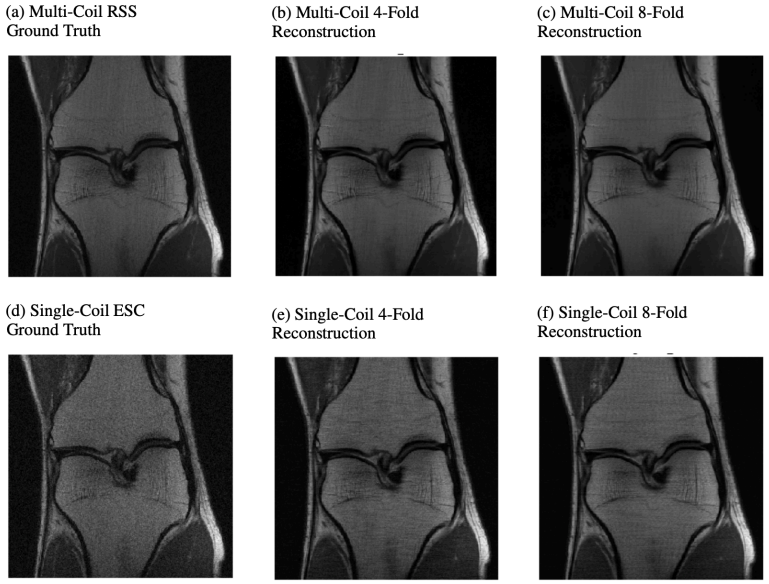




Patrick Putzky
(U. Amsterdam)



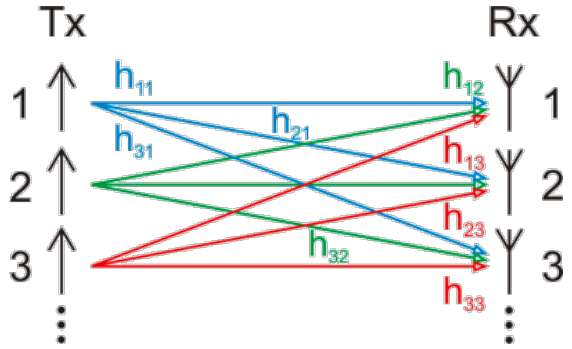
Our neural augmentation implementation (the invertible Recurrent Inference Machine) won the single coil track.



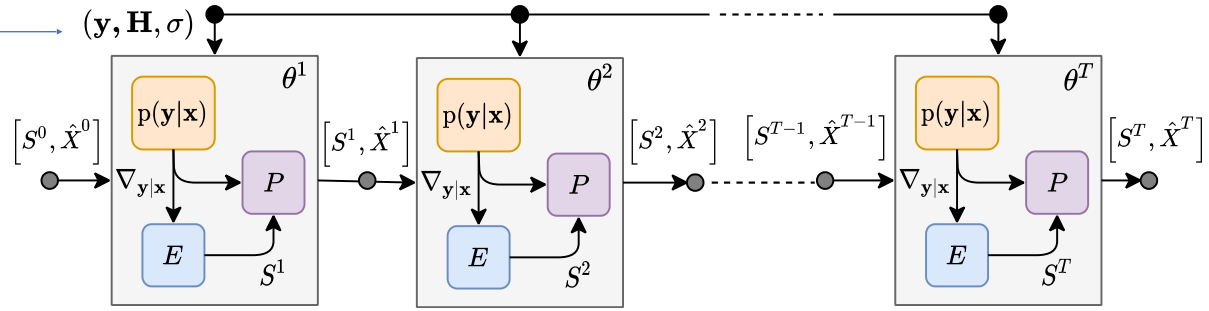
MIMO Detection

Pratik Kumar
(UvA/Qualcomm)

Bhaskar Rao
(UCSD)



MIMO forward model

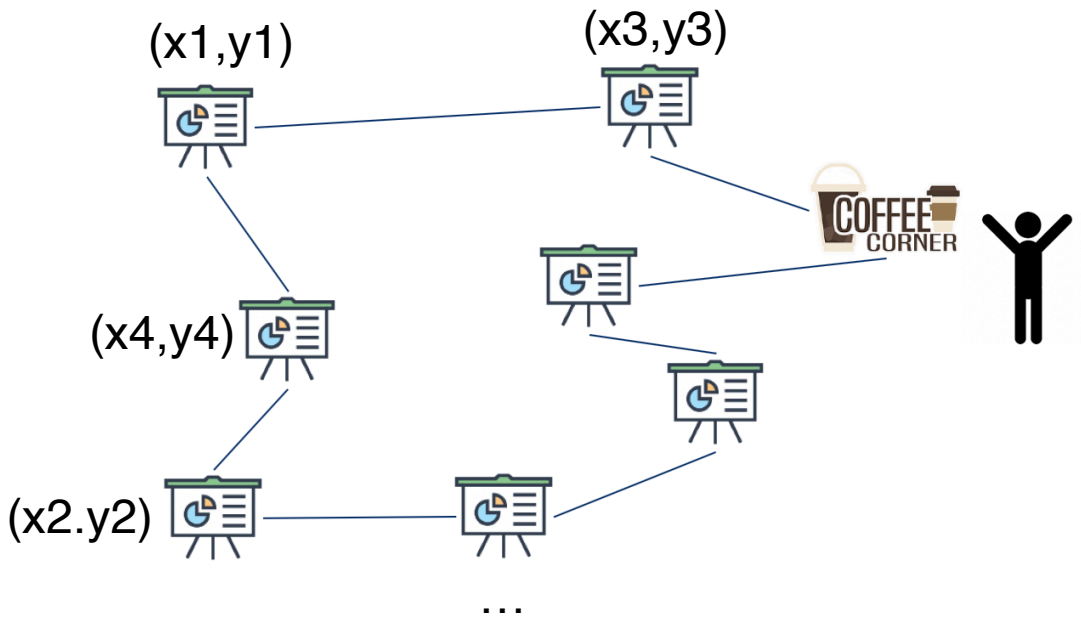


RE-MIMO inverse (inference) model

Amortized Optimization: Traveling Scientist Problem

(Kool et al , ICLR 2019)

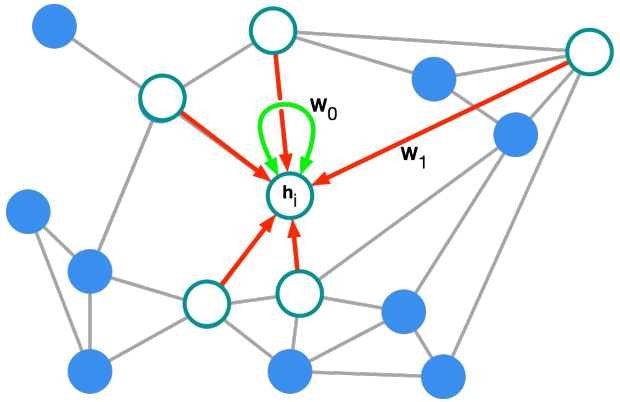
Wouter Kool



Learn Policy $\pi(a|s) \Rightarrow P(\text{next node is } i|\text{previous nodes})$

by generating lots of example trajectories

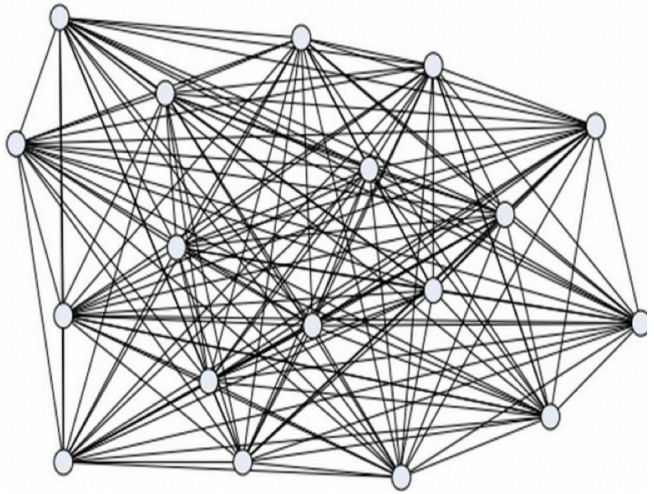
Graph NN



Input as (fully connected) graph

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

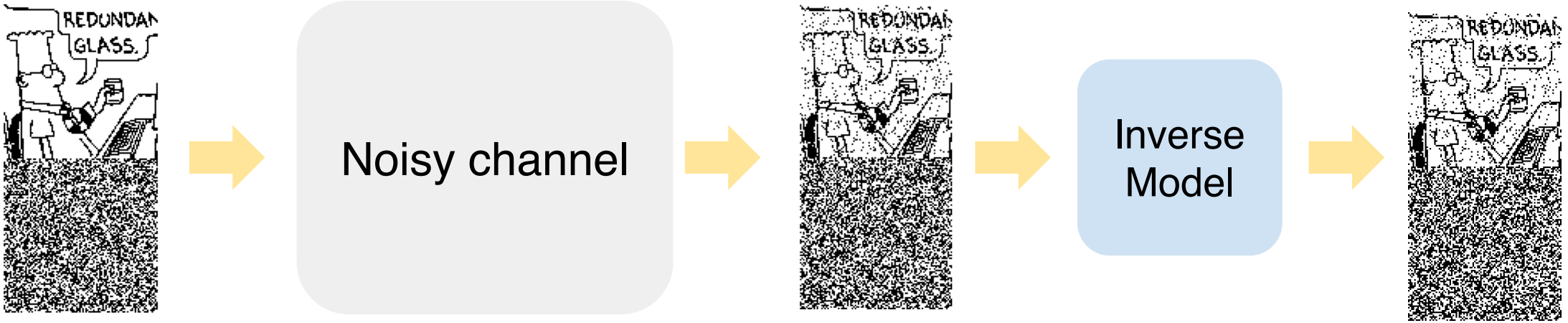
=



Error Correction Decoding

Victor Garcia
(Bosh-UvA Delta Lab

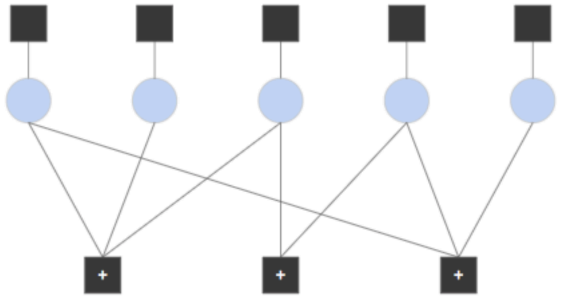
Low Density Parity Check Codes (LDPC)



(Image source: David MacKay)

Neural Augmented Belief Propagation

Factor Graph:



Roll BP out as an RNN

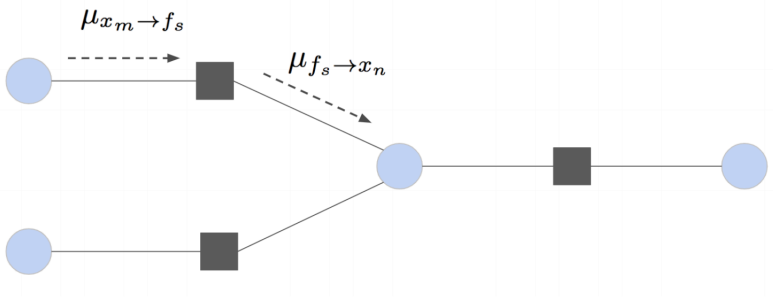


Figure 1. Belief Propagation on a Factor Graph

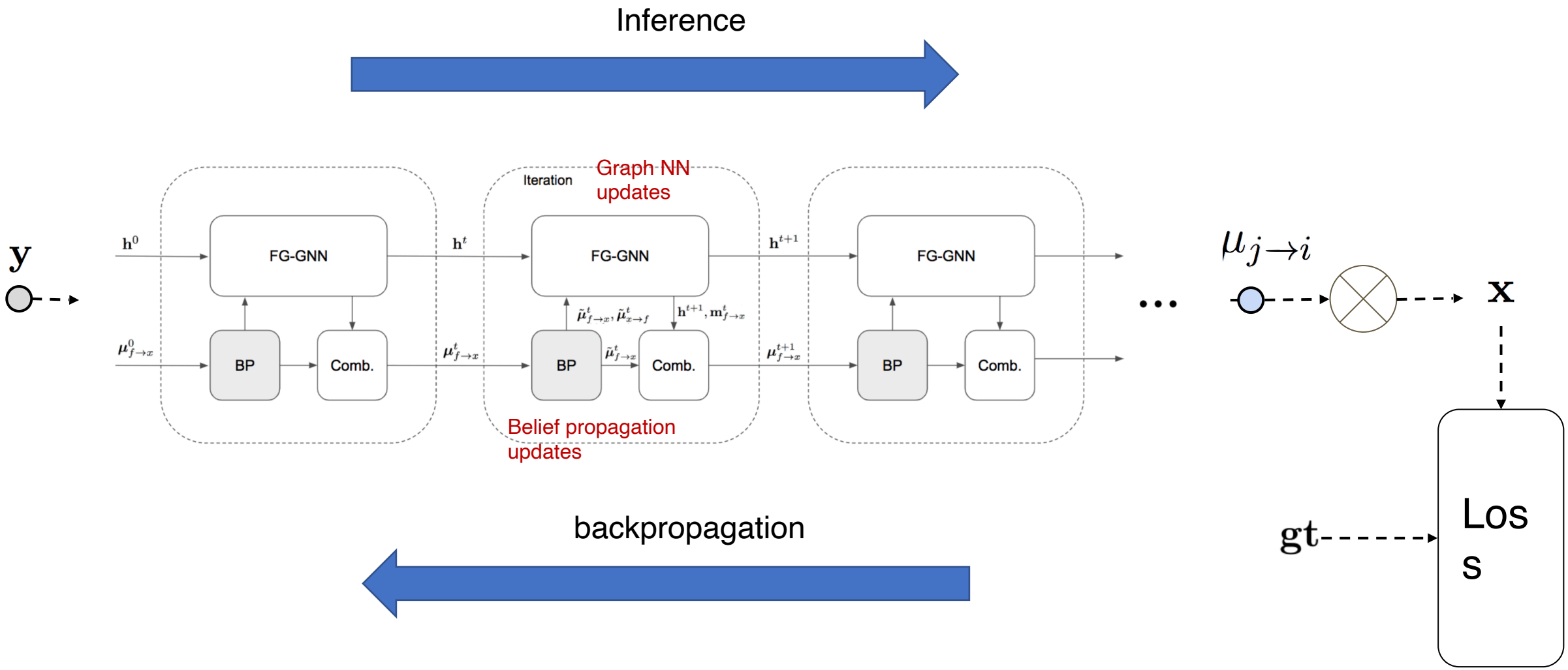
$$\mu_{x_m \to f_s}(x_m) = \prod_{l \in \mathcal{N}(x_m) \setminus f_s} \mu_{f_l \to x_m}(x_m)$$

$$\mu_{f_s \to x_n}(x_n) = \sum_{\mathbf{x}_s \setminus x_n} f_s(\mathbf{x}_s) \prod_{m \in \mathcal{N}(f_s) \setminus n} \mu_{x_m \to f_s}(x_m)$$

$$p(x_n) = \prod_{s \in \mathcal{N}(x_n)} \mu_{f_s \to x_n}(x_n)$$

Graphical Recurrent Inference Network

(Garcia & W. 2020)

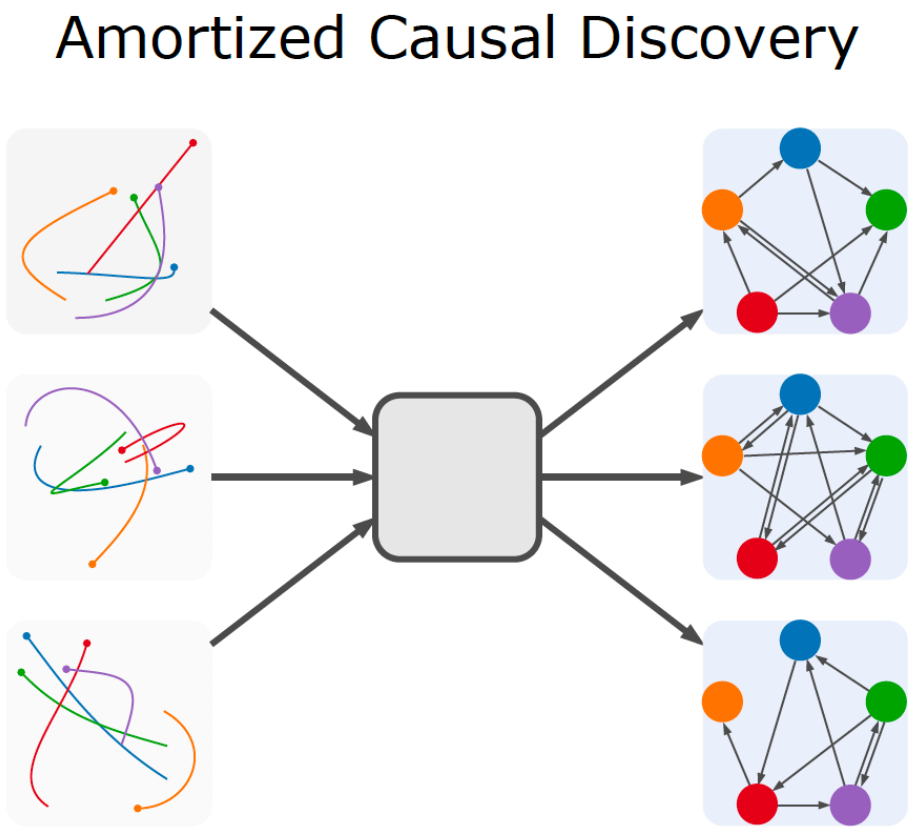


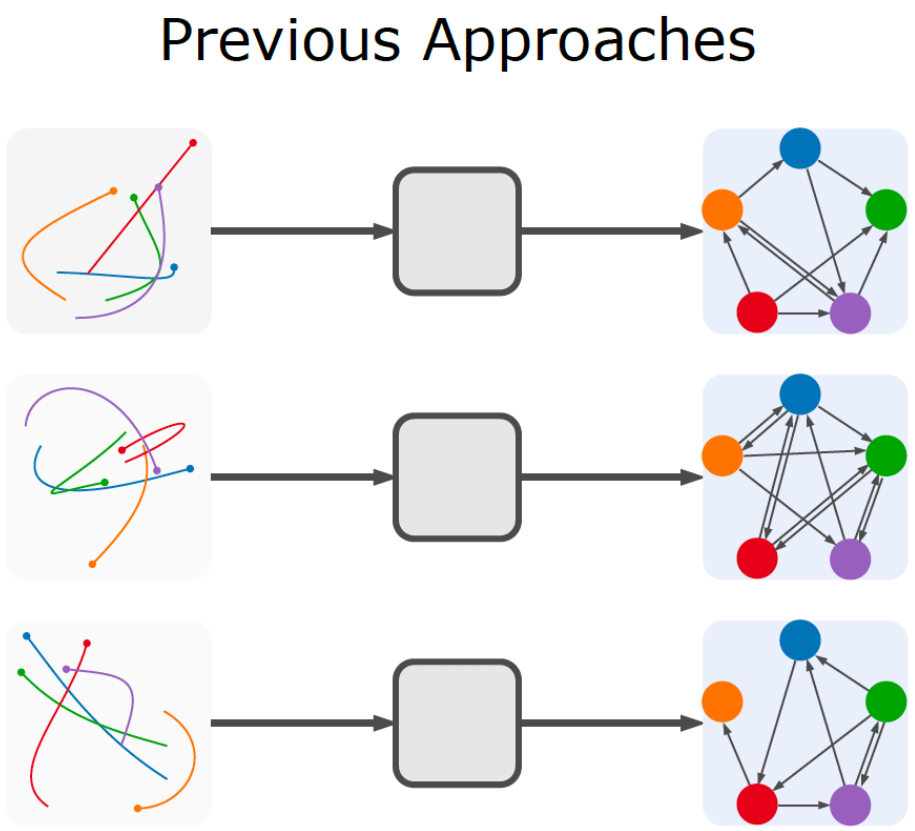
Amortized Causal Discover


Sindy Löwe


David Madras

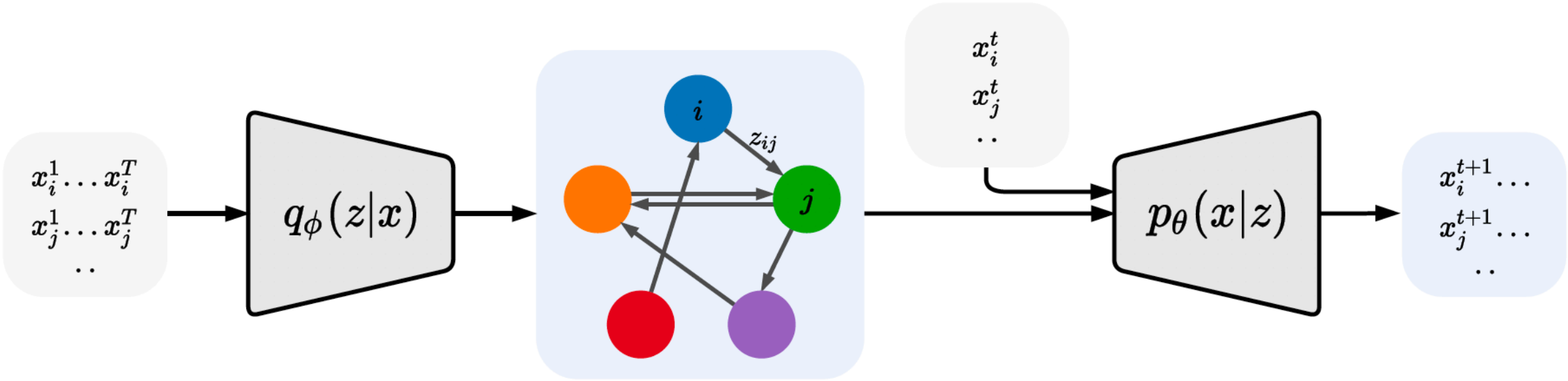

Rich Zemel





Amortized Causal Discovery

ELBO: $\mathcal{L} = \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})] - \mathrm{KL}[q_\phi(\boldsymbol{z}|\boldsymbol{x})||p(\boldsymbol{z})]$



Encoder: $q_\phi(\boldsymbol{z}|\boldsymbol{x}) = \prod q_\phi(\boldsymbol{z}_{ij}|\boldsymbol{x})$

$$z_{ij,e} = GNN(\{x_i^t\}, i = 1..N, t = 1..T)$$

Decoder: $p_\theta(\boldsymbol{x}|\boldsymbol{z}) = \prod_{t=1}^{T} p_\theta(\boldsymbol{x}^{t+1}|\boldsymbol{x}^{\leq t}, \boldsymbol{z})$

$$h_{ij}^t = \begin{cases} 0 & \text{if } z_{ij,0} = 1 \\ \sum_e z_{ij,e} f_e([x_i^t, x_j^t]) & \text{else} \end{cases}.$$

$$\boldsymbol{\mu}_j^{t+1} = \boldsymbol{x}_j^t + f_v\left(\left[\sum_{i \neq j} h_{ij}^t, \boldsymbol{x}_j^t\right]\right)$$

$$p_\theta(\boldsymbol{x}_j^{t+1}|\boldsymbol{x}^t, \boldsymbol{z}) = \mathcal{N}(\boldsymbol{\mu}_j^{t+1}, \sigma^2 \mathbb{I})$$

Conclusions

- Humans seem to continuously predict the future.
- We are surprised when we fail to predict the future correctly: this provides a learning signal
- Are we learning an encoder – decoder pair?
- The encoder is **amortized** for fast prediction and leverages previous inferences
- The encoder is **augmented** generative decoder that helps it correct mistakes real time.
- Two design principles: amortization and augmentation

TL;DR

ThisPersonDoesNotExist.com uses AI generate endless fake faces

Hit refresh to lock eyes with another imaginary stranger

By James Vincent | Feb 15, 2019, 7:38am EST

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A few sample faces — all completely fake — created by ThisPersonDoesNotExist.com