Flow Matching for Solving Inverse Problems

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We present a new way of solving inverse problems using generative modeling with flow matching. Flow Matching opens the door to training generative model with non-diffusion probability paths. These paths are more efficient than diffusion paths, provide faster training and sampling, and result in better generalization. Using flow matching, we can obtain the distribution of possible solutions when the solution to the inverse problem is non-unique.

Flow Matching for solving inverse problems

Suppose we have a forward model

$$d = \mathbf{F}(m, e) + \eta,$$

- Sample m – model parameters.
- Sample e – experiment details.
- Sample noise η from noise distribution
- Compute $d = f(m, e) + \eta$ – experiment design.

These are samples from the **joint distribution** $\rho(d, m, e)$. The model parameter m is not uniquely defined, but has a certain conditional distribution $\rho(m|d, e)$. Our goal is to estimate this distribution. We will use conditional flow matching for this procedure.

Then, we create conditional path between (m_0, d, e) and (m, d, e), where (d, m, e) is from our dataset as

$$m_t = (1 - t)m_0 + t\ \ m, \quad t\ \ [0, 1].$$

In conditional flow matching, we need to learn velocity $v_\theta(m_t, t, d, e)$ that minimizes the following loss function:

$$\mathbf{E}_{t, m_0, (m,d,e)\ \ p}\ \ v_\theta(m_t, t, d, e) - (m - m_0)\ ^2 \rightarrow \min_\theta$$

$$\frac{dm_t}{dt} = v(m_t, t, d, e), \quad m_t(0) = m_0.$$

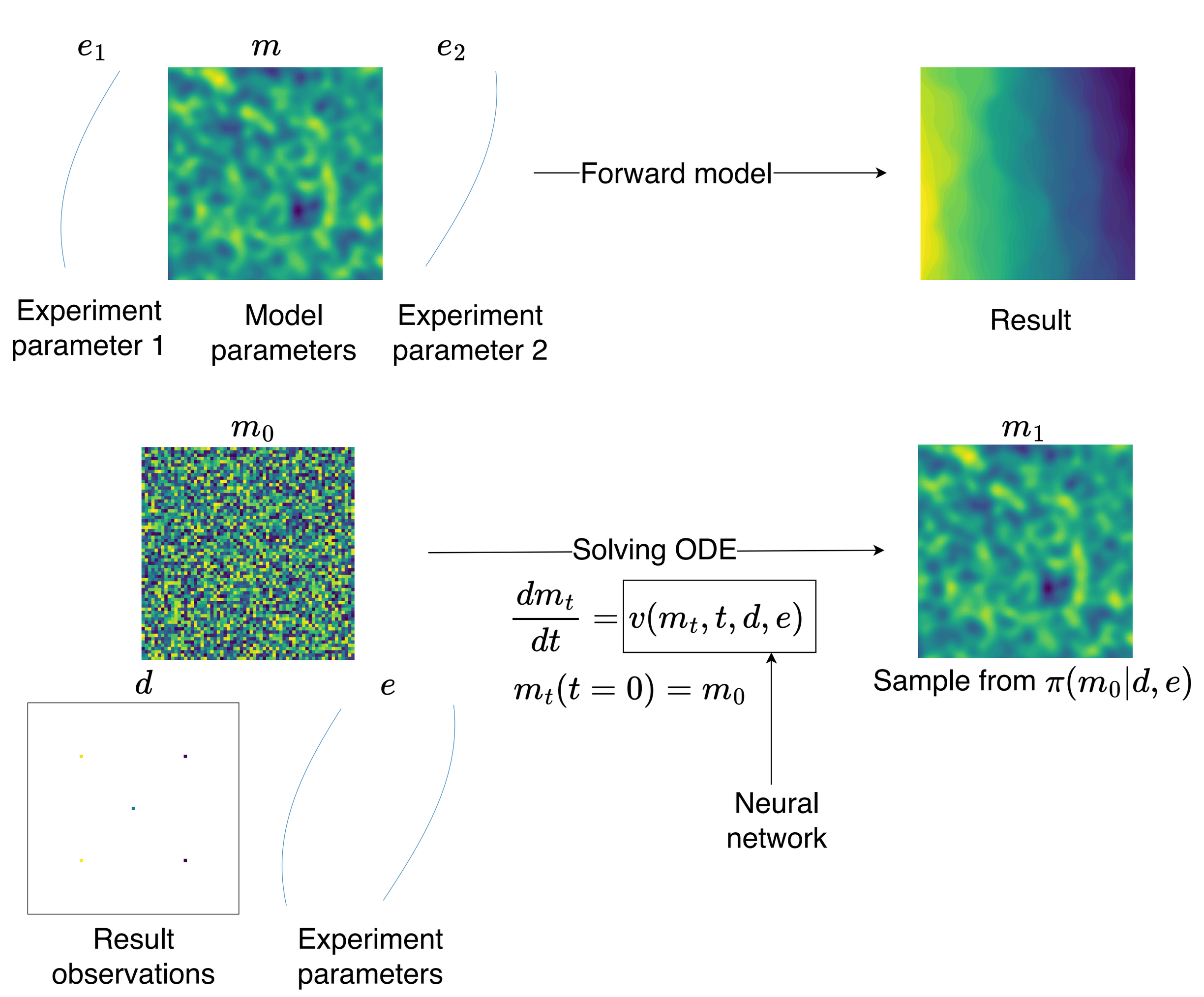

Figure 1. Solving the inverse problem using flow-matching

SEIR disease model

SEIR (Susceptible-Exposed-Infected-Recovered) model is a mathematical model used to mathematically simulate the spread of infectious diseases. In this case study we simulate a real situation where, during the spread of a disease, we measure the number of infected and dead people at random times and use this information to try to recover the control parameters of the ODE system.

$$\frac{dS}{dt} = -\beta(t)SI, \frac{dE}{dt} = \beta(t)SI - \alpha E$$

$$\frac{dI}{dt} = \alpha E - \gamma(t)I, \frac{dR}{dt} = \gamma(t)I$$

where the variables $S(t)$ is susceptible number, $E(t)$ is exposed number, $I(t)$, $R(t)$ are infected and removed number initialized with $S(0) = 99$, $E(0) = 1$, $I(0) = R(0) = 0$.

$$\beta(t) = \beta_1 + \frac{\tanh(7(t - \tau))}{2}(\beta_2 - \beta_1)$$

$$\gamma(t) = \gamma^r + \gamma^d(t); \gamma^d(t) = \gamma_1^d + \frac{\tanh(7(t - \tau))}{2}(\gamma_2^d - \gamma_1^d)$$

i.e., the rates transition smoothly from some initial rate (β_1 and γ_1^d) to some final rate (β_2 and γ_2^d) around time $\tau > 0$. We fix $\tau = 2.1$ and an overall time interval of $[0, 4]$.

- $e = [a_1, a_2, a_3, a_4]\ \ \mathbf{U}[1, 3]$ random times, when measurements are performed
- $d_i = [I_{e_i}, R_{e_i}]$ for $i\ \ [1, 4]$ ($d\ \ \mathbf{R}^{2\times 4}$) the number of infected and deceased individuals
- $m = [\beta_1, \alpha, \gamma^r, \gamma_1^d, \beta_2, \gamma_2^d]$ is ODE model parameters.

Assume $m_{\mathbf{true}} = [0.4, 0.3, 0.3, 0.1, 0.15, 0.6]$. Then after 1000 calculations the average error will be $2.05\% \pm 1.04\%$.

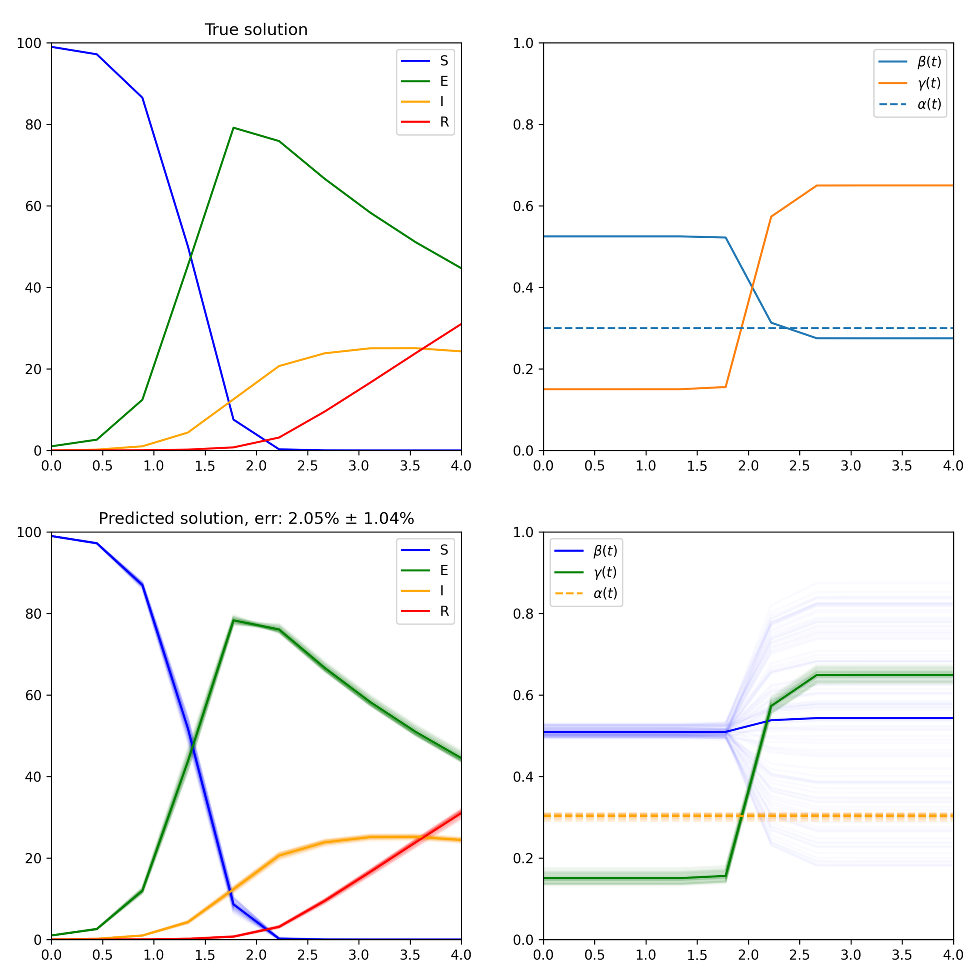

Figure 2. Probabilistic solutions to the inverse problem

Permeability field inversion

In this example, the inverse problem consists of estimating the spatially-dependent diffusivity field κ, given measurements of the pressure u at some pre-determined locations $(x_i, y_i)\ \ \Omega$. This is a common problem, for example in the oil industry, when there are a small number of wells and pressure observations across them, and from these data one needs to reconstruct the permeability field of an oil field.

$$-\ \ \cdot (\kappa\ \ u) = 0$$

with boundary conditions

$$u(x = 0, y) = f(y, e_1) = \exp\left(-\frac{1}{2\sigma_w}(y - e_1)^2\right)$$

$$u(x = 1, y) = g(y, _2) = -\exp\left(-\frac{1}{2\sigma_w}(y - e_2)^2\right)$$

κ is the spatially-dependent diffusivity field given measurements of the pressure u at some pre-determined locations $(x_i, y_i)\ \ \Omega$. $m = \log(\kappa)\ \ N(0, C_{pr})$, with covariance operator C_{pr}

$$c(x, z) = \sigma_v^2 \exp\left[\frac{-\ \ x - z\ \ ^2}{2\ell^2}\right] \quad \text{for } x, z\ \ \Omega,$$

with $\sigma_v = 1$ and $\ell^2 = 0.1$. Employing a truncated Karhunen-Loève expansion of the unknown diffusivity field yields the approximation

$$m(x, \mathbf{m}) \approx \sum_{i=1}^{n_m} m_i \sqrt{\lambda_i}\phi_i(x),$$

where λ_i and $\phi_i(x)$ denote the i-th largest eigenvalue and eigenfunction of C_{pr}, $m_i\ \ N(0, 1)$. The Karhunen-Loève expansion is truncated after $n_m = 16$ modes, resulting in an approximation that captures 99 percent of the weight of C_{pr}.

- m is a 16 parameters for Karhunen-Loève expansion of log-permeability of field
- $e = [e_1, e_2]$ Dirichlet boundary conditions coefficients
- d is 3, 4, 5 or more u observations in fixed points.

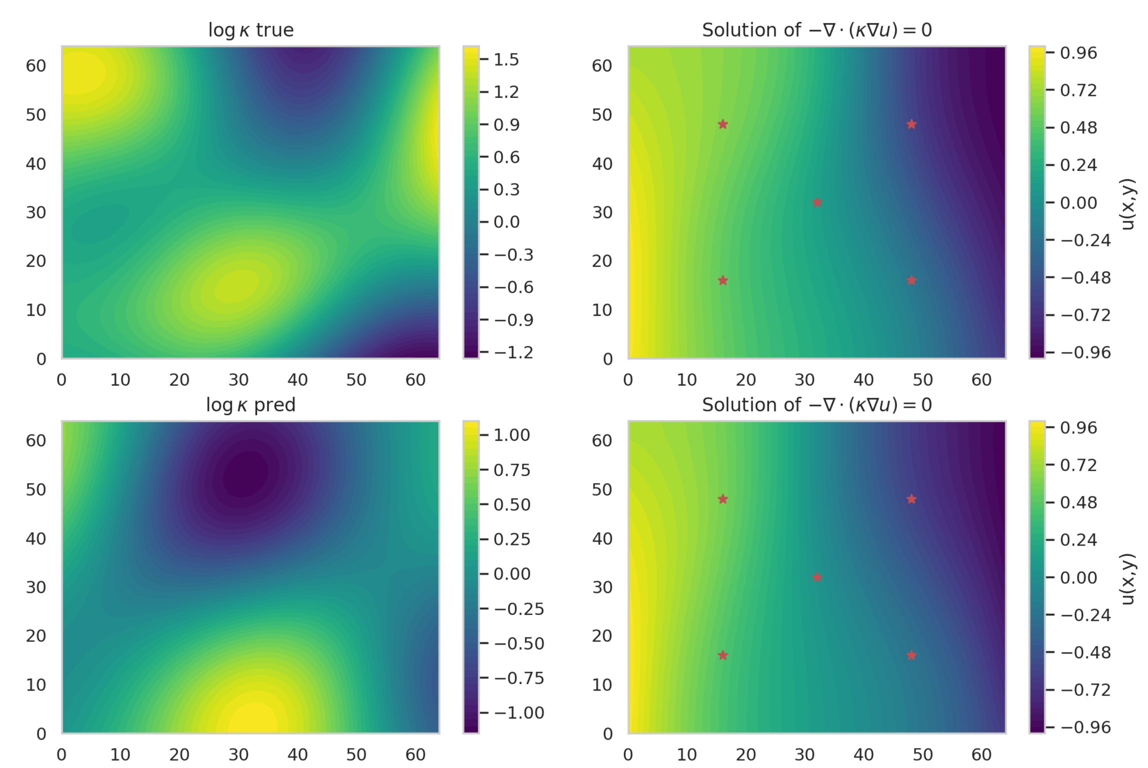

Figure 3. Probabilistic solutions to the inverse problem

Simple nonlinear model

In our experiments, we used the following forward model from [Koval et al.]

$$d(e, m) = e^2 m^3 + m \exp(-|0.2 - e|) + \eta$$

where the η is a known noise distribution, i.e. $\mathbf{N}(0, \sigma^2)$. In the simplest example in Koval et al., m – model parameter is one dimensional, uniformly distributed on $[0, 1]$. Also, e is one-dimensional from $[0, 1]$ (input point, 'experiment'), we can also take it uniformly distributed on $[0, 1]$.

$$m_0\ \ \mathbf{U}[0, 1].$$

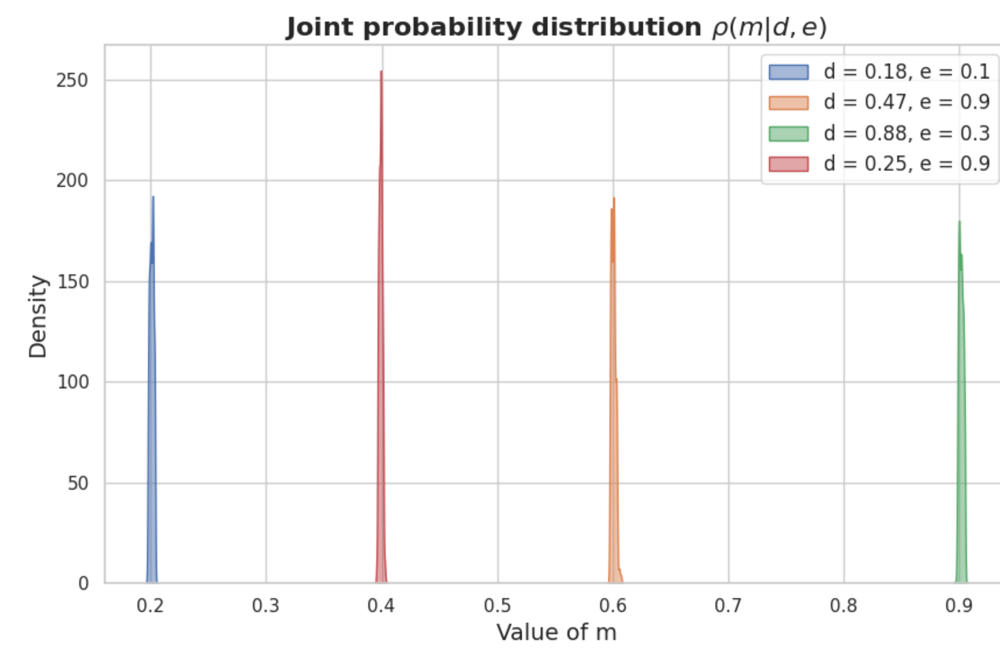

Figure 4. Joint probability of m parameter visualisation for different design d and experiments e parameters

Conclusions

For different cases of inverse problem solving, the following results are obtained:

Case	Mean d error, %	std. d error, %
Simple nonlinear	0.15	0.09
SEIR ODE system	2.04	1.01
Pressure diffusivity PDE*	0.81	0.53

Table 1. Inverse problem solution results.

* - for 5 point case.

References

[1] Karina Koval, Roland Herzog, and Robert Scheichl. Tractable optimal experimental design using transport maps, 2024.

[2] Yaron Lipman, Ricky T. Q. Chen, Heli Ben-Hamu, Maximilian Nickel, and Matt Le. Flow matching for generative modeling, 2023.