Analysis of the Stochastic Inverse Problem

Maria Oprea

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Joint work with Qin Li (UW Madison), Li Wang (UMN Twin Cities) and Yunan Yang (Cornell)

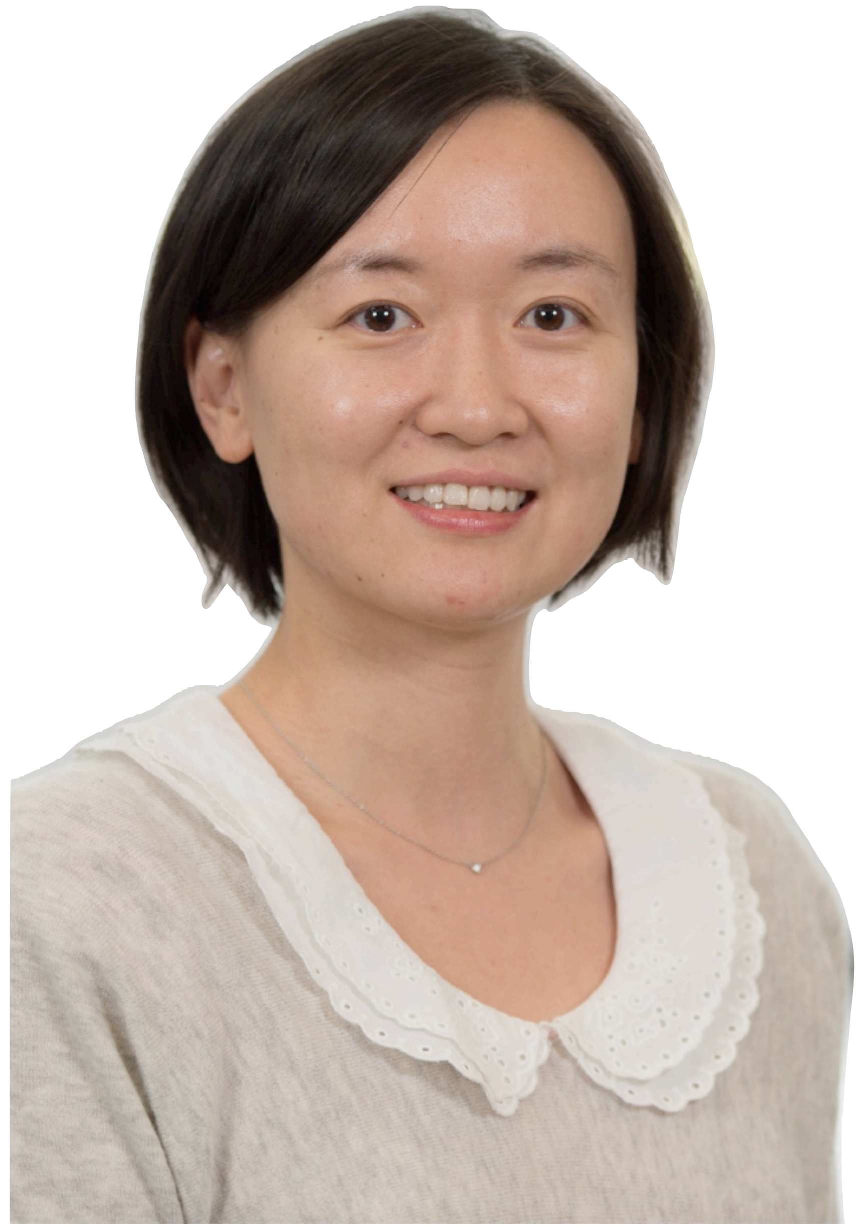
Stochastic Inverse Problem: stability, regularization and Wasserstein gradient flow, Qin Li, O., Li Wang, Yunan Yang, arxiv:2410.00229

Collaborators

Qin Li

UW Madison

Li Wang



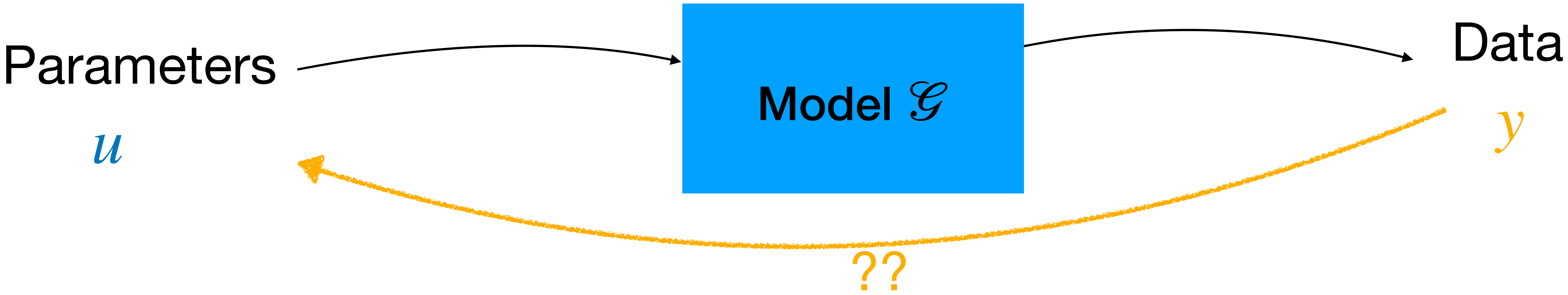
UM Twin Cities

Yunan Yang

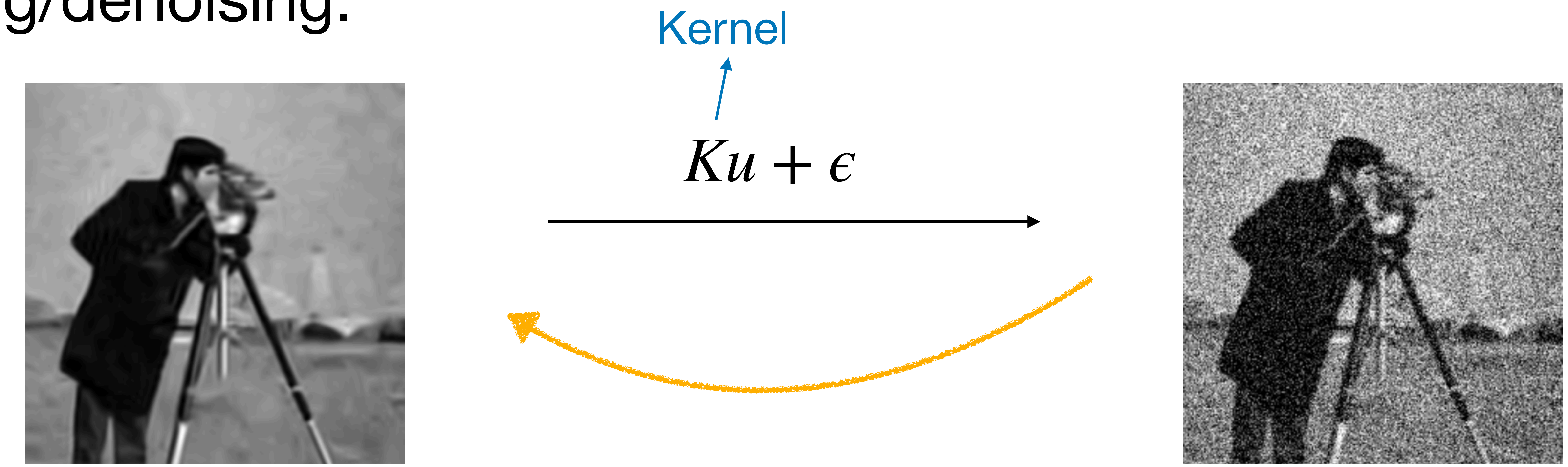
Cornell University

Qin Li, O., Li Wang and Yunan Yang, Stochastic Inverse problem: Stability, Regularization and Wasserstein Gradient Flow, preprint

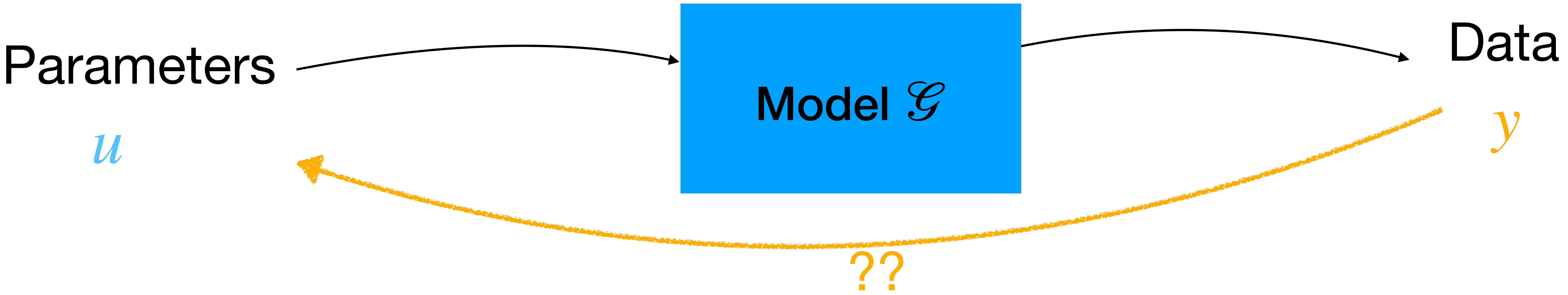
Inverse problems



- Some examples: - training a NN
  - $\mathscr{G}(u)$ = solution to $\nabla \cdot (u(x)\nabla y(x)) = 0, x \in \Omega$ with Dirichlet boundary conditions
  - Image deblurring/denoising:



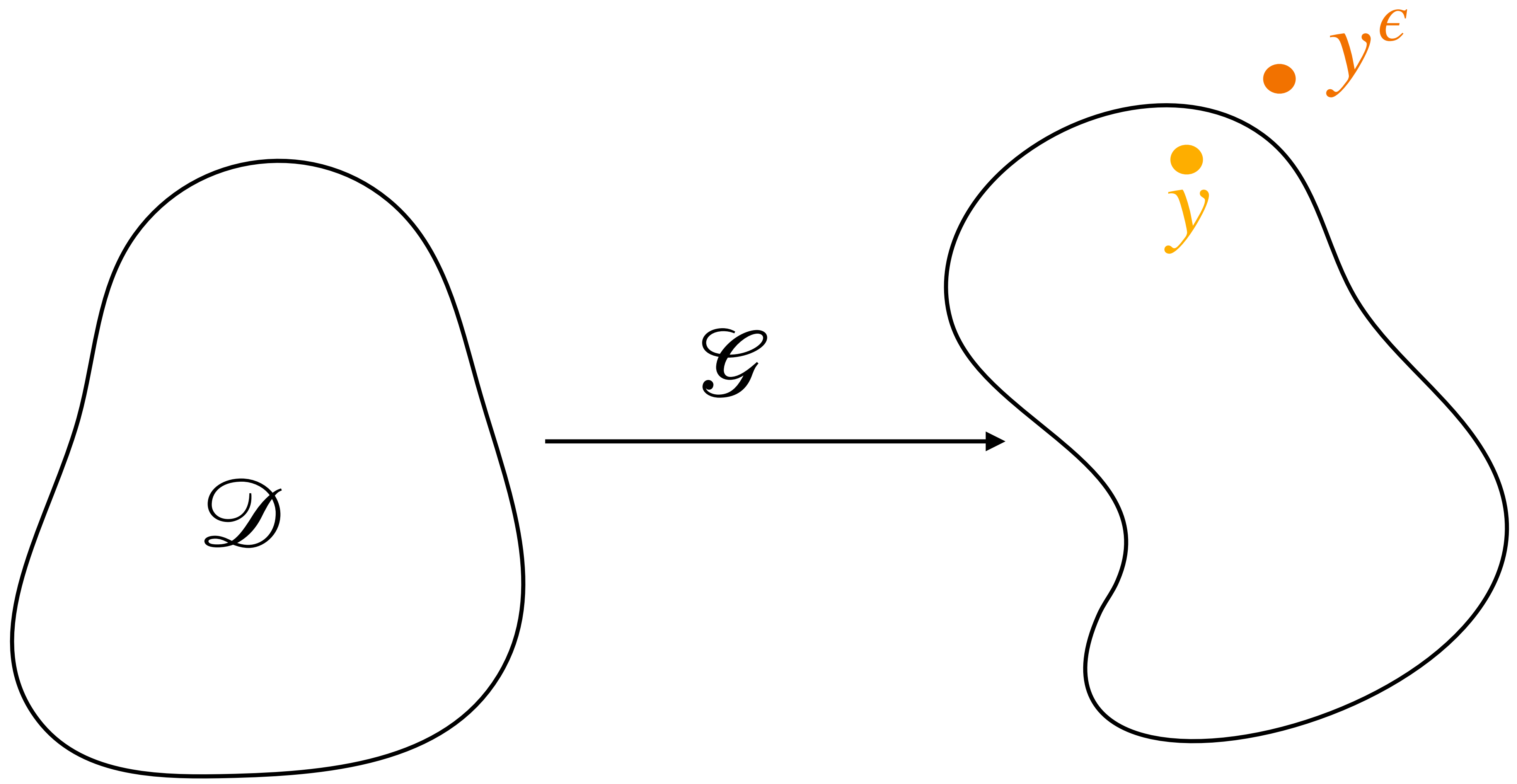
Inverse problems



- Naive idea: $u = \mathscr{G}^{-1}(y)$

  - ✖ $\mathscr{G}$ might not be invertible
  - ✖ Data is noisy $y^{\epsilon} = y + \epsilon$
  - ✖ $y^{\epsilon} \notin \mathscr{G}(\mathscr{D})$
  - ✖ Inversion might not be stable

    $\|\mathscr{G}^{-1}(y) - \mathscr{G}^{-1}(y^{\epsilon})\|_{\mathscr{D}}$ large



Regularization and Gradient Flows

- Reformulate as an optimization problem $\min_{u \in \mathcal{D}} \|\mathcal{G}(u) - y\|_{\mathcal{R}}$

Norm in $\mathcal{R}$

- Add regularization: $\min_{u \in \mathcal{D}} L(u) = \min_{u \in \mathcal{D}} \|\mathcal{G}(u) - y\|_{\mathcal{R}} + \mathrm{R}(u)$

Promote sparsity/smoothnes

- How to solve: gradient descent method $u_{n+1} = u_n - \alpha \nabla L(u_n)$

$$\Big\Downarrow \text{ Continuous time}$$

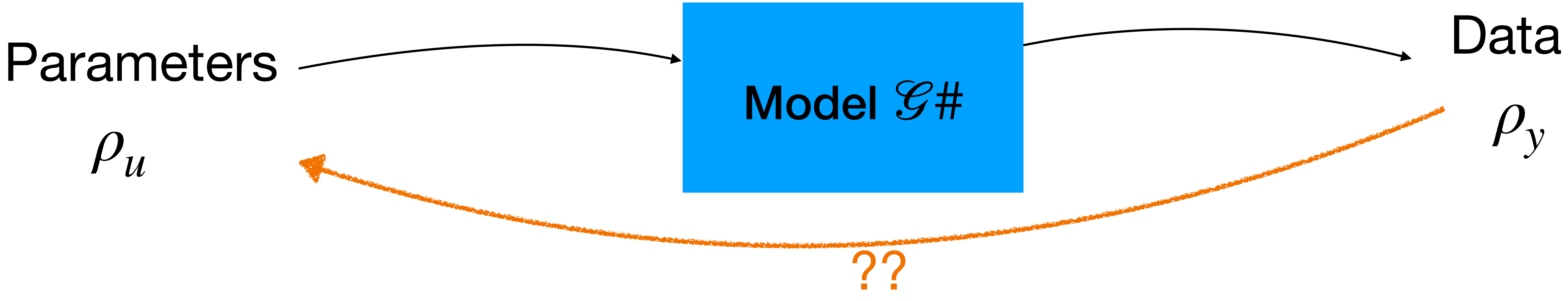
$$\dot{u} = -\nabla_u L(u)$$

Depends on the choice of metric!

- As $t \to \infty$, $u(t) \to u_0$, a minimizer of $L(u)$

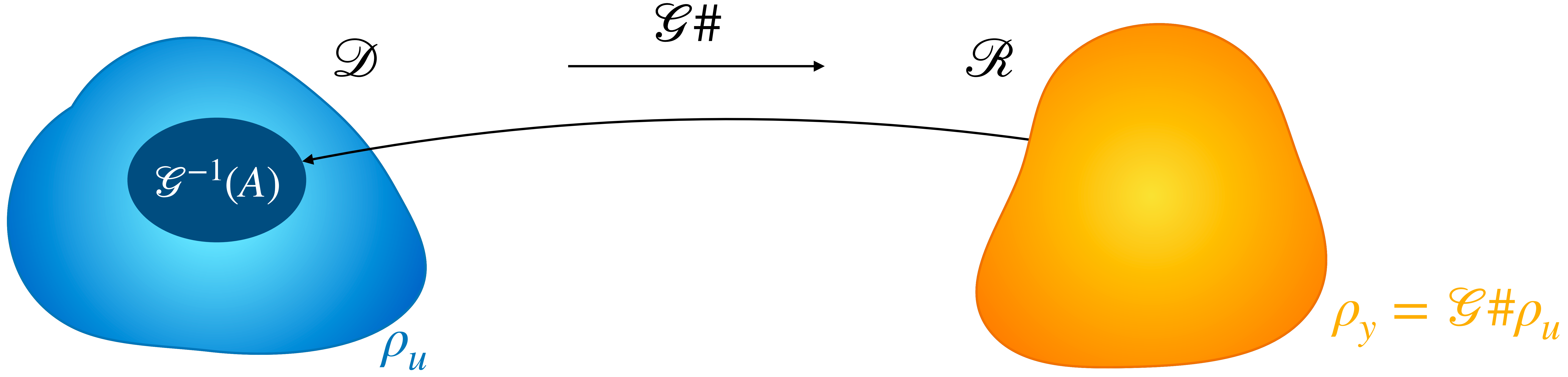
Stochastic inverse problem

- What if the parameter is a distribution?



Definition: If $\mathscr{G} : \mathscr{D} \to \mathscr{R}$ then $\mathscr{G}\# : \mathscr{P}(\mathscr{D}) \to \mathscr{P}(\mathscr{R})$ such that $\mathscr{G}\#\mu(A) = \mu(\mathscr{G}^{-1}(A))$

$X \sim \mu \implies \mathscr{G}(X) \sim \mathscr{G}\#\mu$



Stochastic inverse problem

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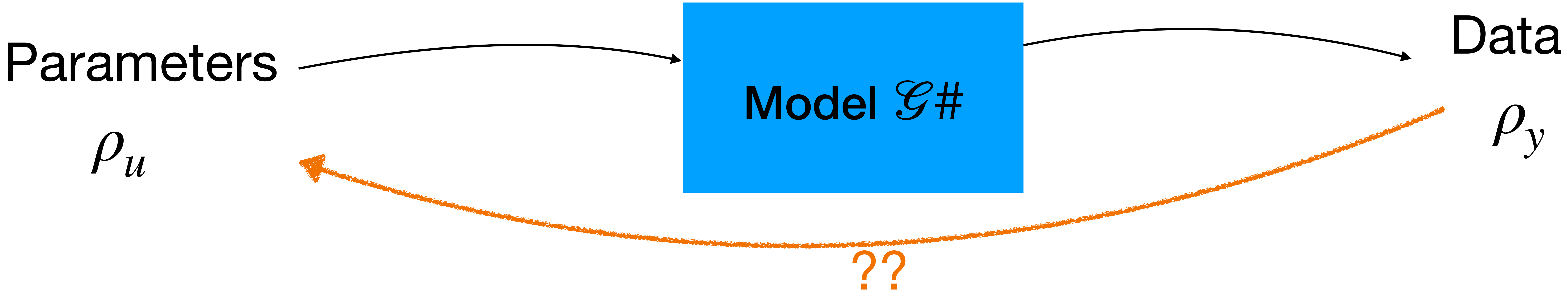
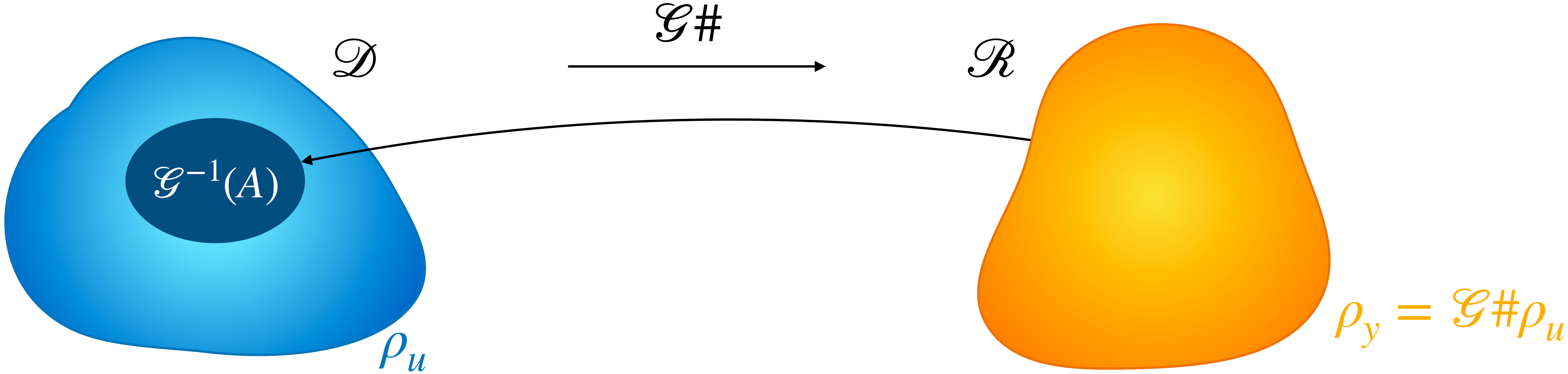
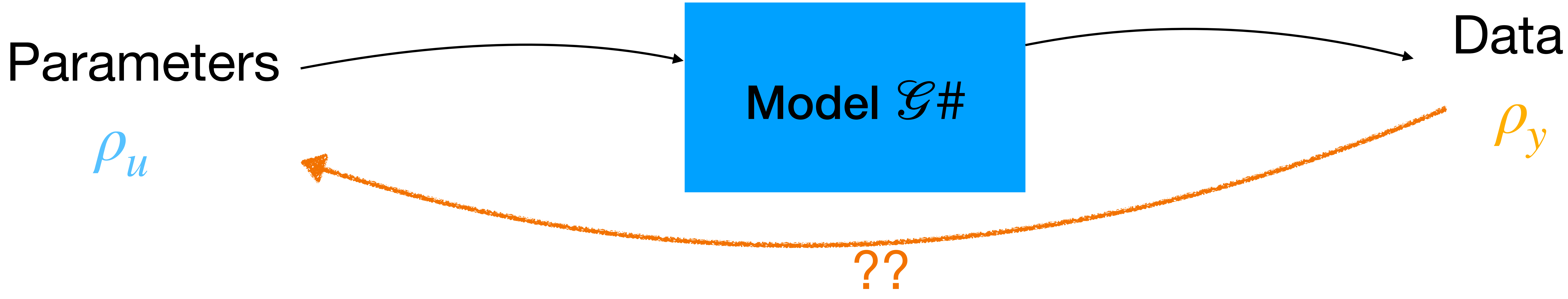


$$X \sim \mu \implies \mathscr{G}(X) \sim \mathscr{G}\#\mu$$



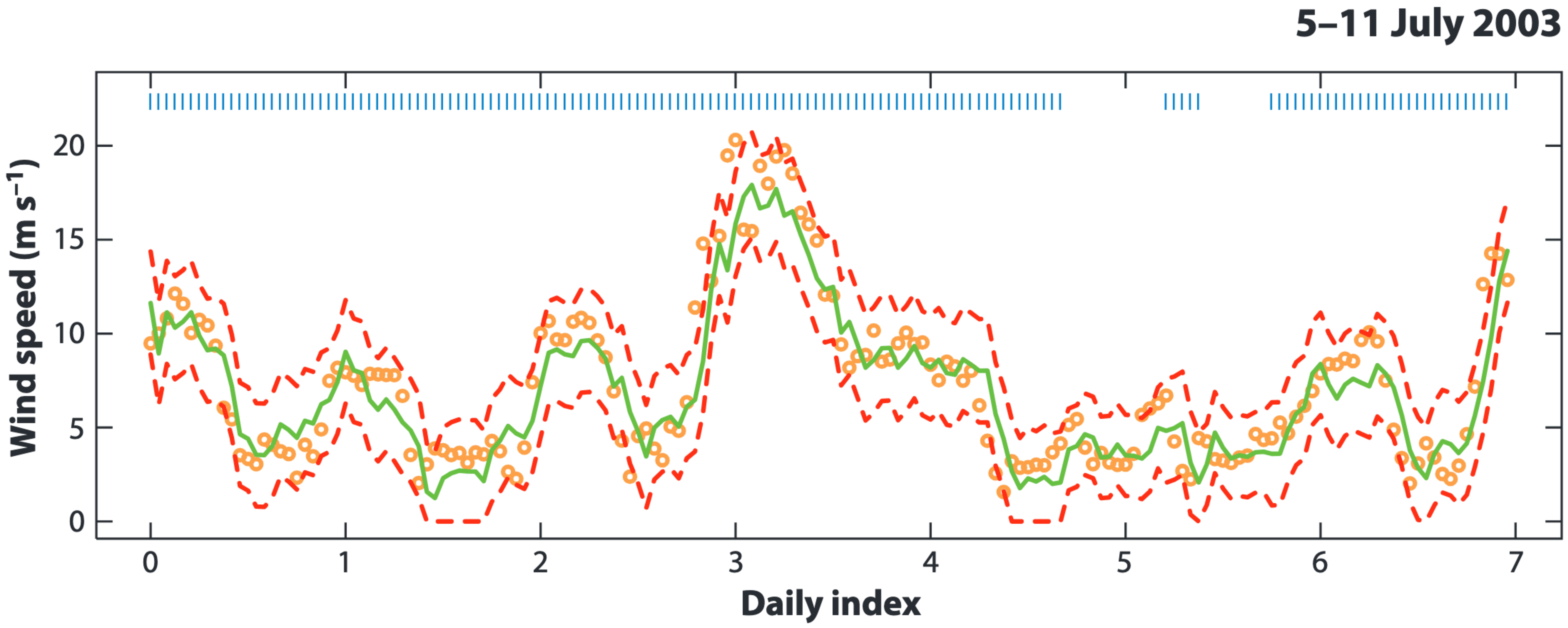
Stochastic inverse problem



- Questions for the rest of the talk:
  - ? How to understand $(\mathscr{G}\#)^{-1}(\rho_y)$? Stability? General $\mathscr{G}$ if invertible, linear under-determined
  - ? What does the variational framework look like? Linear system with W_2 regularizer
  - ? What is the performance of the gradient flow solver? Linear over-determined

Motivation

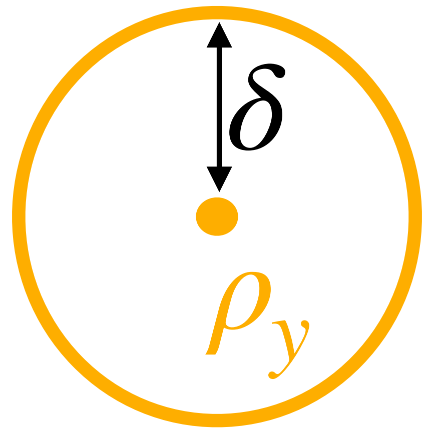
- Repeated measurements $\Longrightarrow$ different results
- Data itself is a distribution: cryoEM, climate modeling, plasma



T. Gneiting and M. Katzfuss, Probabilistic forecasting, Annual Review of Statistics and Its Application, 1 (2014), pp. 125–151

Spaces and norms

- $\rho_u \in \mathscr{P}(\mathscr{D})$; $\rho_y, \rho_y^\delta \in \mathscr{P}(\mathscr{R})$, ρ_y^δ is in the δ ball of ρ_y



measured distribution

- Metrics:

  - Wasserstein distance: $W_p(\mu, \nu) = \left(\inf_{\pi \in \Gamma(\mu,\nu)} \int \|x - y\|_p d\pi \right)^{\frac{1}{p}} \rightarrow \mathscr{P}_p$

  - f divergence $D_f(\mu \| \nu) = \int f\left(\frac{d\mu}{d\nu}\right) d\nu \rightarrow \mathscr{P}_{ac}$

    Ex: KL, χ^2, TV, …

Stochastic Inverse problem

Can be empirical

Goal: Given polluted data ρ_y^δ and the deterministic model, find the parameter distribution ρ_u^δ such that the distance between the true distribution ρ_u and the computed one ρ_u^δ is as small as possible

?

$\longleftarrow$

Direct inversion, linear case

- Assume $\mathcal{G} := A : \mathbb{R}^n \to \mathbb{R}^m$ linear.

- When A is invertible: $(A\#)^{-1} = A^{-1}\#$

Theorem: If $\rho_u = A^{-1}\#\rho_y$ **and** $\rho_u^\delta = A^{-1}\#\rho_y^\delta$ **then:**

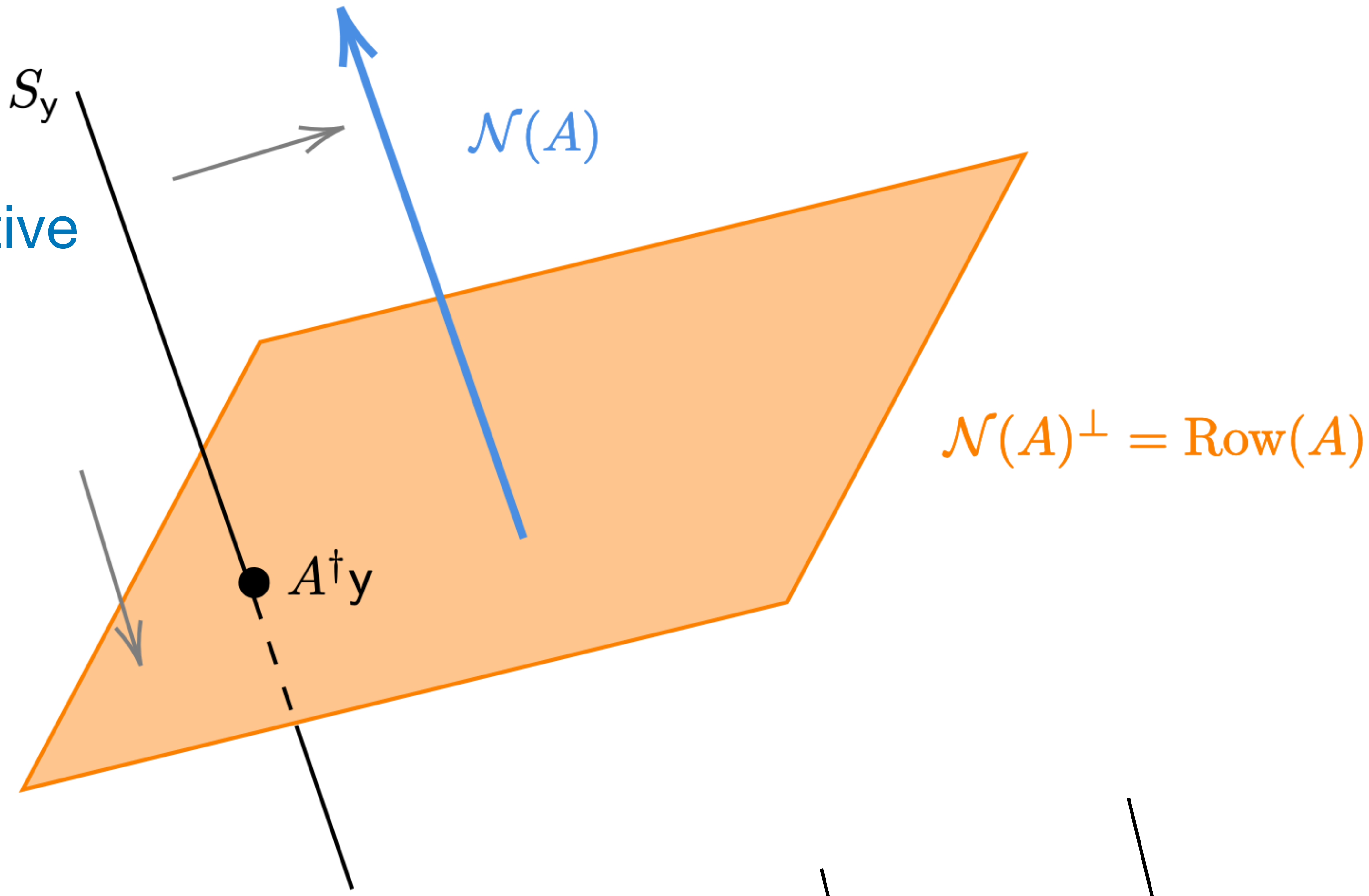
- $W_p(\rho_u, \rho_u^\delta) \leq C_{A^{-1}} W_p(\rho_y, \rho_y^\delta)$ with $C_{A^{-1}} = \dfrac{1}{\sigma_{min}(A)}$
- $D_f(\rho_u \| \rho_u^\delta) = D_f(\rho_y \| \rho_y^\delta)$

Better stability!

- When $\boxed{A}$ is over-determined if $supp(\rho_y) \not\subset Col(A)$ then $\nexists \rho_u$ such that $A\#\rho_u = \rho_y$

Under-determined case

Onto, not injective

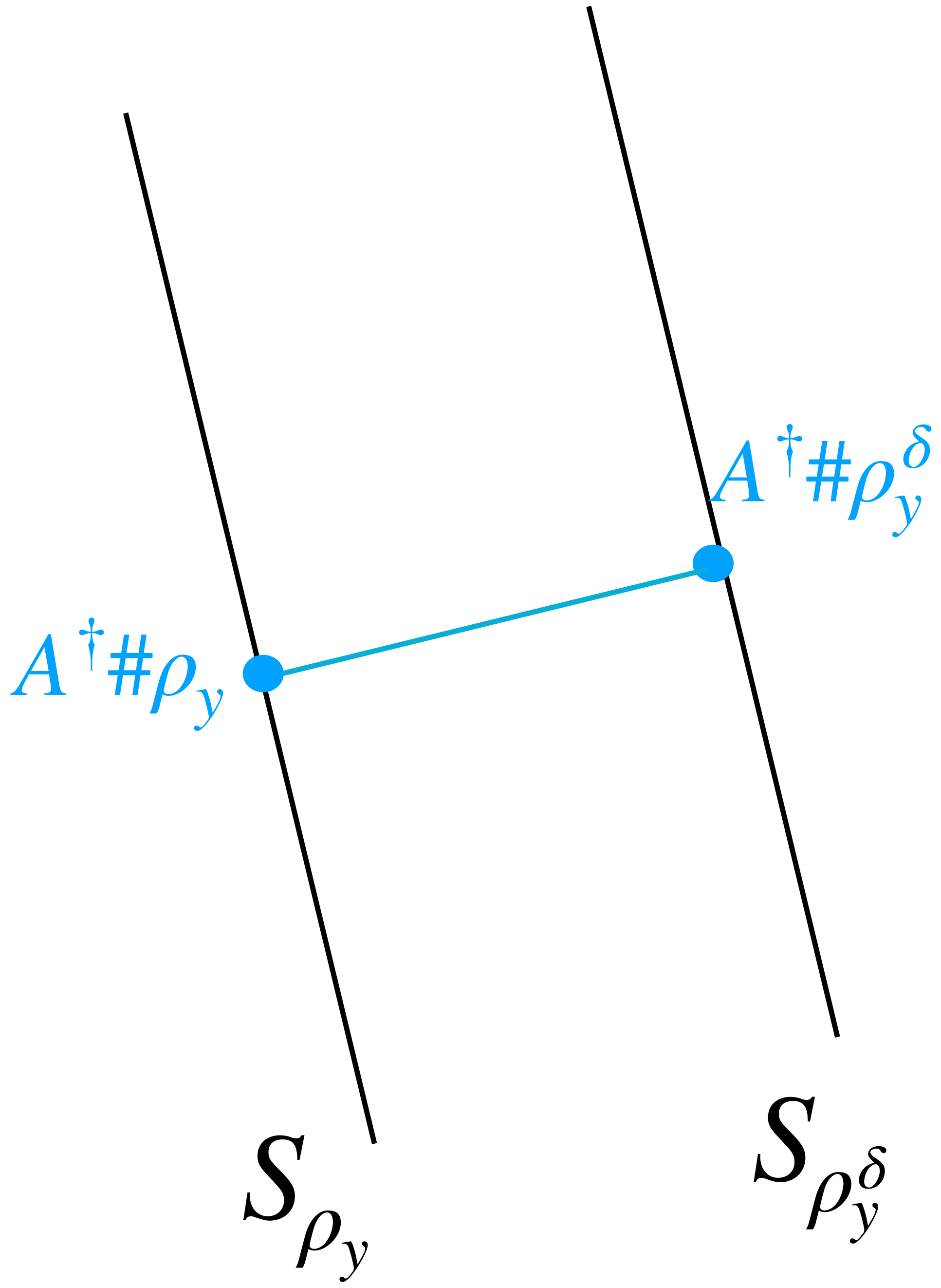


- Solution set $S_{\rho_y} = \{\rho_u \,|\, A\#\rho_u = \rho_y\}$
- Consider the infimum distance

$$d(S_{\rho_y}, S_{\rho_y^\delta}) = \inf_{\substack{\{\mu : A\#\mu = \rho_y^1\} \\ \{\nu : A\#\nu = \rho_y^2\}}} d(\mu, \nu)$$

Theorem: if $\boxed{\textbf{A}}$ has full row rank

- $d^W(S_{\rho_y}, S_{\rho_y^\delta}) = W_2(A^{\dagger}\#\rho_y, A^{\dagger}\#\rho_y^\delta) \le (\sigma_{min}(A))^{-1} W_2(\rho_y, \rho_y^\delta)$ **with**
- $d^f(S_{\rho_y} \| S_{\rho_y^\delta}) = D_f(\rho_y \| \rho_y^\delta)$



- Sup distance $\to \infty$

Variational Framework with regularization

$$\rho_u^\delta = \text{arg} \min_{\rho_u \in \mathscr{P}(\mathscr{D})} E[\rho_u; \rho_y^\delta] := \text{arg} \min_{\rho_u \in \mathscr{P}(\mathscr{D})} D(\mathscr{G}\#\rho_u, \rho_y^\delta) + \alpha \mathrm{R}(\rho_u)$$

- $W_2 - W_2$ pair: $D = W_2$ and $\mathrm{R}(\rho_u) = \underbrace{\int |u|^2 d\rho_u}_{W_2^2(\rho_u, \delta_0)}$

Theorem: If $\mathscr{G} = \boxed{A}$ linear with full column rank then:

- If $\alpha = \delta = 0$ then $\rho_u^* = A^\dagger \# \rho_y$ is the minimizer
- Else, $(\rho_u^\delta)^* = (A^\top A + \alpha^2 \mathrm{I})^{-1} A^\top \# \rho_y^\delta$ is the minimizer

Tikhonov regularization in probability space!

Wasserstein Gradient Flow

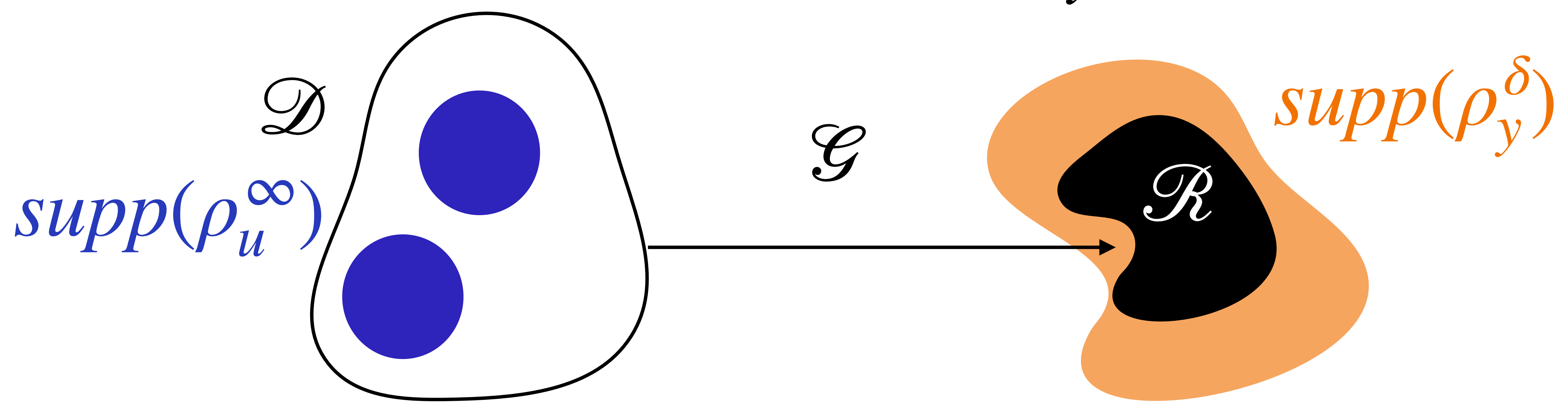
- Treat the case of Wasserstein gradient flow $\partial_t \rho_u = \nabla \cdot \left(\rho_u \nabla \frac{\delta E}{\delta \rho_u} \right)$

- Case 1. Of KL divergence: $D = D_f$

Theorem: Let $\rho_y^\infty = \mathscr{G}\#\rho_u^\infty$ **(equilibrium of the GF), then** $\frac{\rho_y^\infty}{\rho_y^\delta}(\mathscr{G}(u)) = C$ **on connected components of** $supp(\rho_u^\infty)$**. If** $supp(\rho_y^\delta) = \mathscr{R}$ **then** $\rho_y^\infty = \rho_y^\delta$

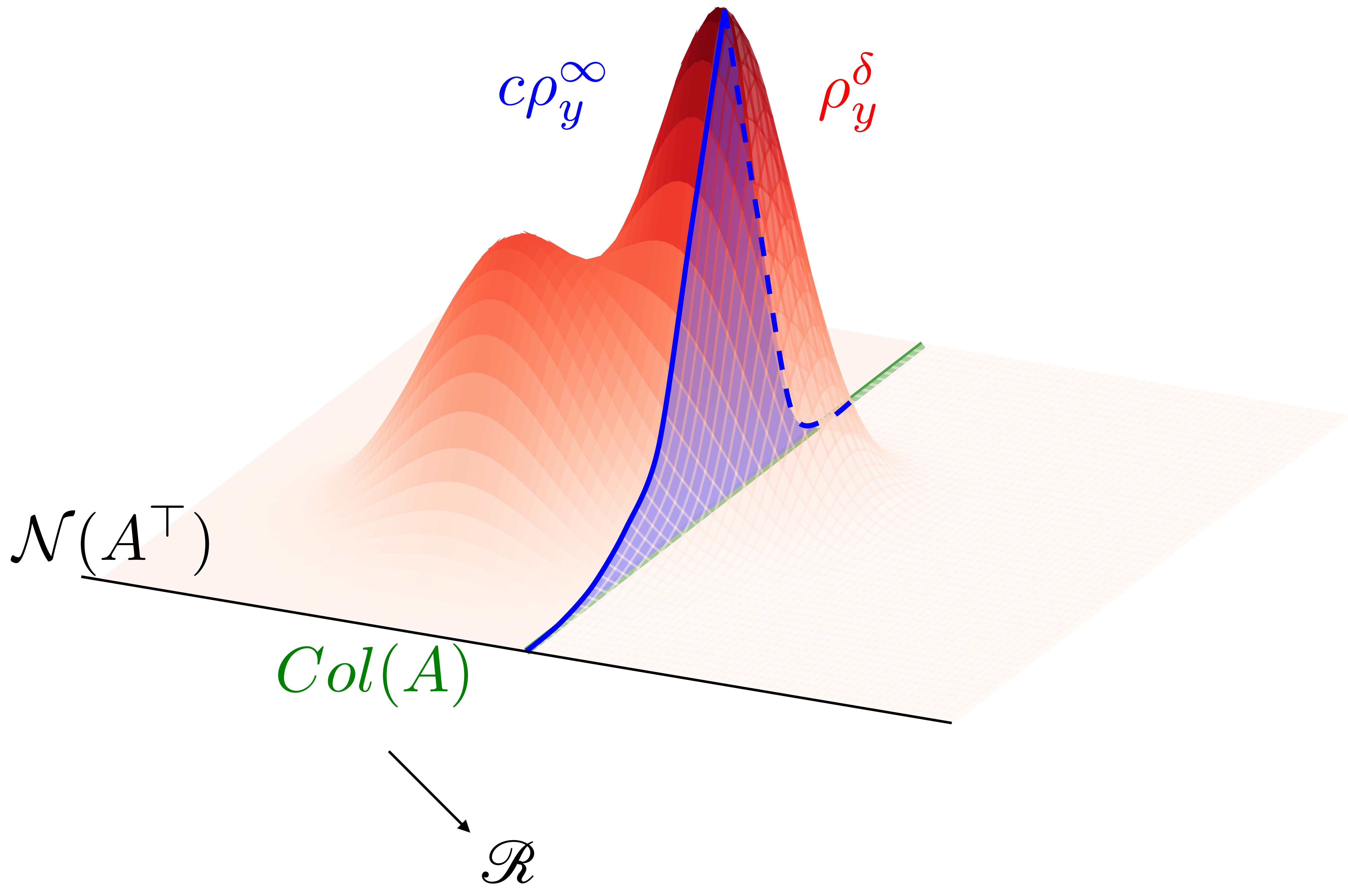
If $\mathscr{R} \subset supp(\rho_y^\delta)$ **then** $\rho_y^\infty = \rho_y^\delta | \mathscr{R}$

- If $\mathscr{G} = A$ linear and over-determined then ρ_y^∞ is the conditional distribution of ρ_y^δ on $Col(A)$



Wasserstein Gradient Flow of KL divergence

- If $\mathscr{G} = A$ linear and over-determined then ρ_y^∞ is the conditional distribution of ρ_y^δ on $Col(A)$

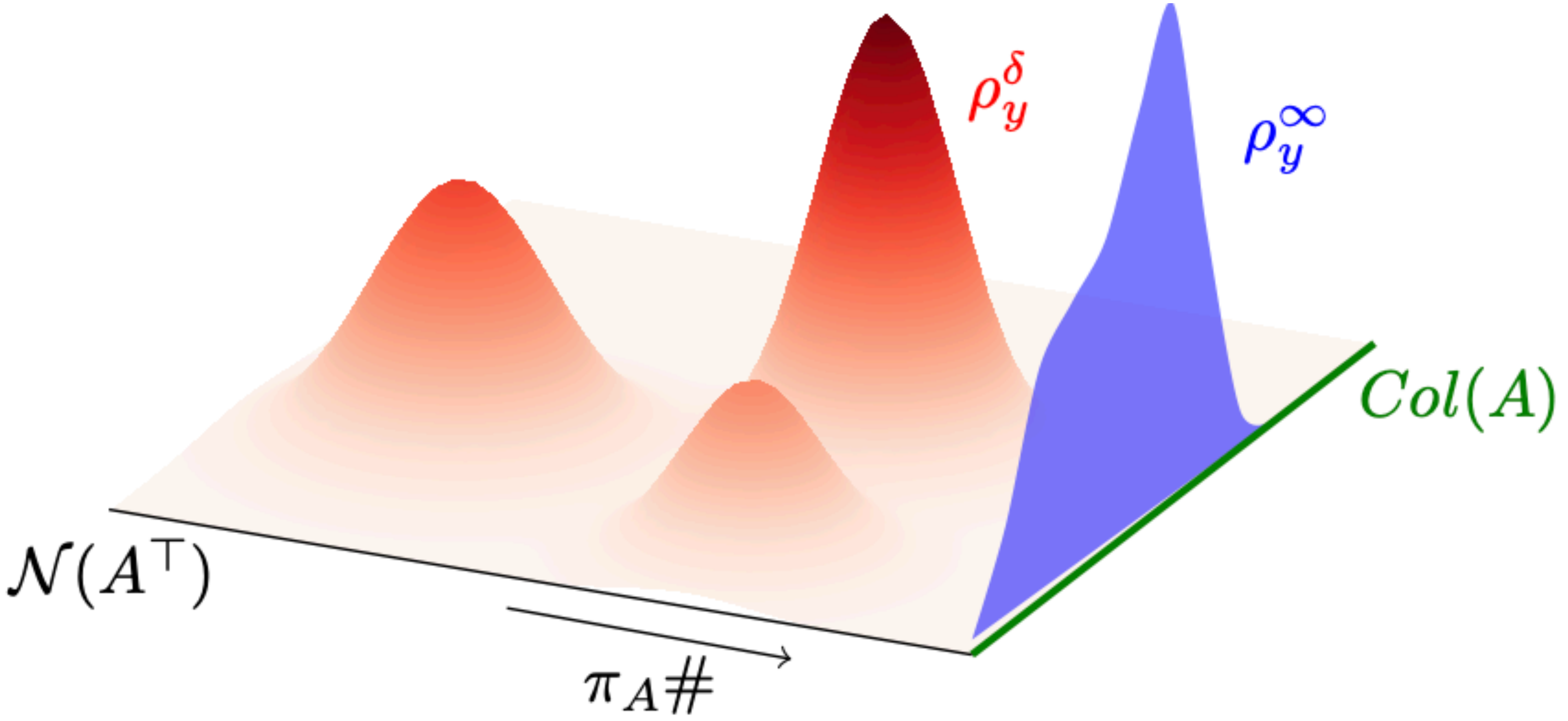


Wasserstein Gradient Flow of W_2

- Case 2. $D = W_2$, consider $\mathscr{G} = A$. Then $\rho_u^\infty = A^\dagger \# \rho_y^\delta$

Projection onto $Col(A)$

- ρ_y^∞ recovers the marginal distribution of ρ_y^δ onto $Col(A)$



Thank you for listening! Questions?

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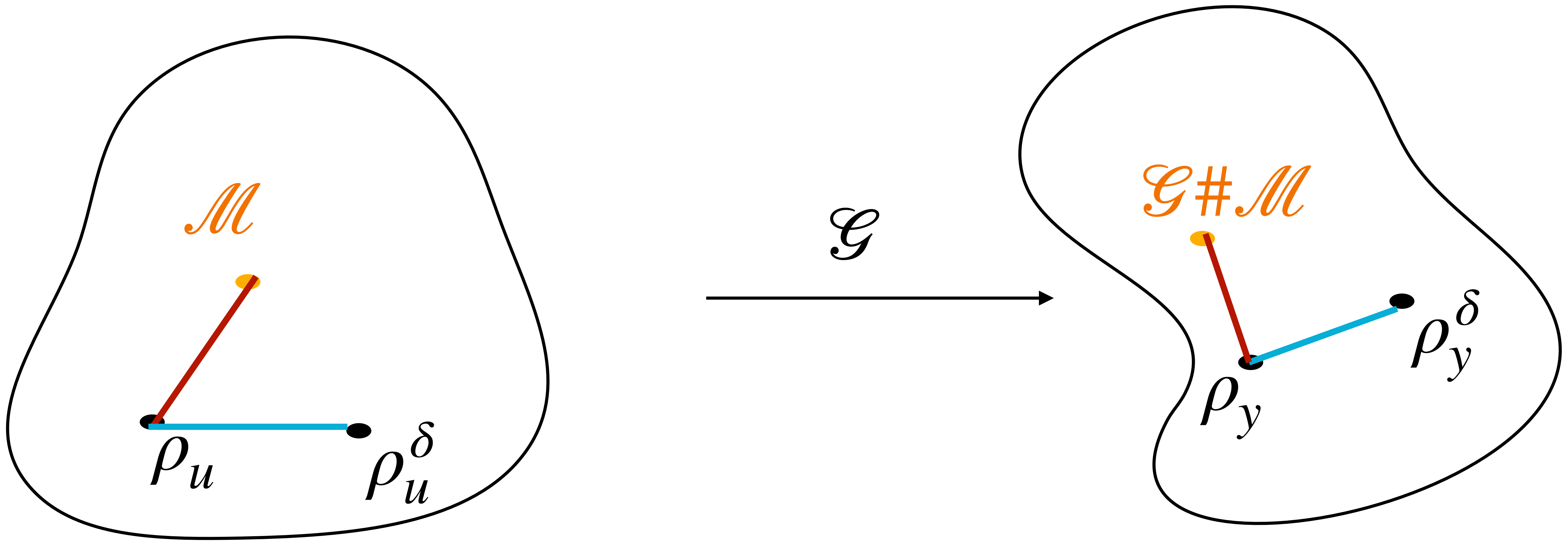
Supplemental slides

- Regularization with Entropy-Entropy pair: $D = KL$ and R $= KL(\cdot \| \mathscr{M})$

Theorem: If $\mathscr{G}$ is invertible then:

- $\rho_u^\delta = C\left(\mathscr{G}^{-1}\#\rho_y^\delta \mathscr{M}^\alpha\right)^{\frac{1}{1+\alpha}}$
- $KL(\rho_u \| \rho_u^\delta) = \dfrac{1}{\alpha+1} KL(\rho_y \| \rho_y^\delta) + \dfrac{\alpha}{\alpha+1} KL(\rho_y \| \mathscr{G}\#\mathscr{M}) - \log C$



Variational Framework with regularization

$$\rho_u^\delta = \arg\min_{\rho_u \in \mathscr{P}(\mathscr{D})} E[\rho_u; \rho_y^\delta] := \arg\min_{\rho_u \in \mathscr{P}(\mathscr{D})} D(\mathscr{G}\#\rho_u, \rho_y^\delta) + \alpha \mathrm{R}(\rho_u)$$

- Existence: if E is l.s.c and coercive

Desired output measure

- Entropy-Entropy pair: $D = KL$ and R $= KL(\cdot \| \mathscr{M})$

Theorem: If $\mathscr{G}$ is invertible then:

- $\rho_u^\delta = C\left(\mathscr{G}^{-1}\#\rho_y^\delta \mathscr{M}^\alpha\right)^{\frac{1}{1+\alpha}}$
- $KL(\rho_u \| \rho_u^\delta) = \dfrac{1}{\alpha+1} KL(\rho_y \| \rho_y^\delta) + \dfrac{\alpha}{\alpha+1} KL(\rho_y \| \mathscr{G}^{-1}\#\mathscr{M}) - \log C$

Exponential convergence

Theorem: If $\mathcal{G} = A$ linear, $D = KL$ and ρ_y^δ is $\lambda-$log concave and $KL(\rho_y(0)||\rho_y^\delta) < \infty$ then $\rho_y(t)$ converges to the conditional distribution $\rho_y^\delta \,|\, Col(A) := \rho_{y_A}^\delta$ exponentially fast in terms of the KL divergence i.e:

$$KL(\rho_y(t)||\rho_{y_A}) \leq exp(-2\lambda\sigma_{min}^2 t)KL(\rho_y(0)||\rho_y^\delta)$$

Proof for KL Wasserstein Gradient Flow

- $$\partial_t \rho_u = \nabla \cdot \left(\rho_u \nabla \frac{\delta E}{\delta \rho_u} \right) \implies \partial_t \rho_y = \nabla_y \cdot \left[\rho_y B(y) \nabla_y \log \left(\frac{\rho_y}{\rho_y^\delta} \right) \right], \quad y \in \mathscr{R}$$

- At equilibrium RHS = 0

$$\frac{\rho_y^\infty}{\rho_y^\delta}(\mathscr{G}(u)) = C$$ on simply connected subsets of supp(ρ_u^∞)