Neural Networks Can Automatically Adapt to Low-Dimensional Structure in Inverse Problems

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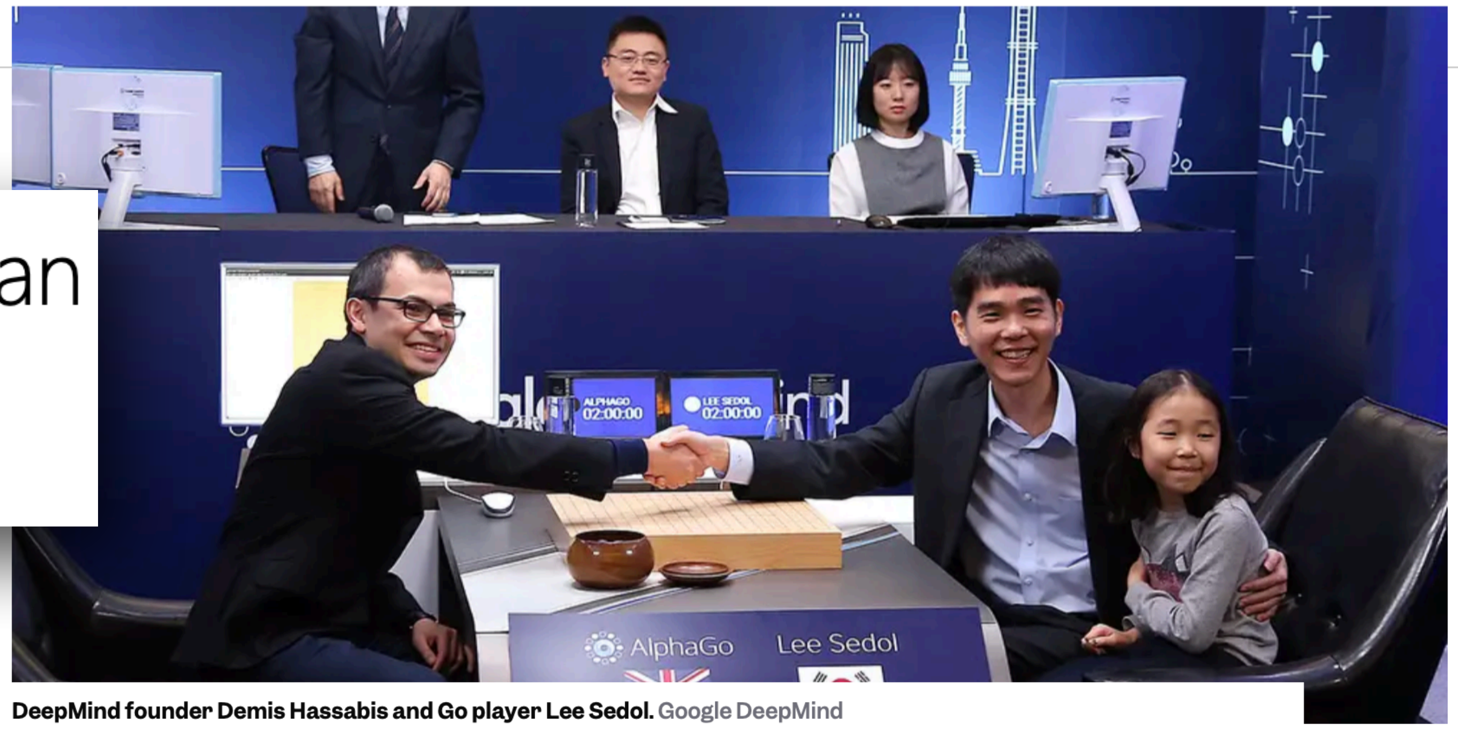

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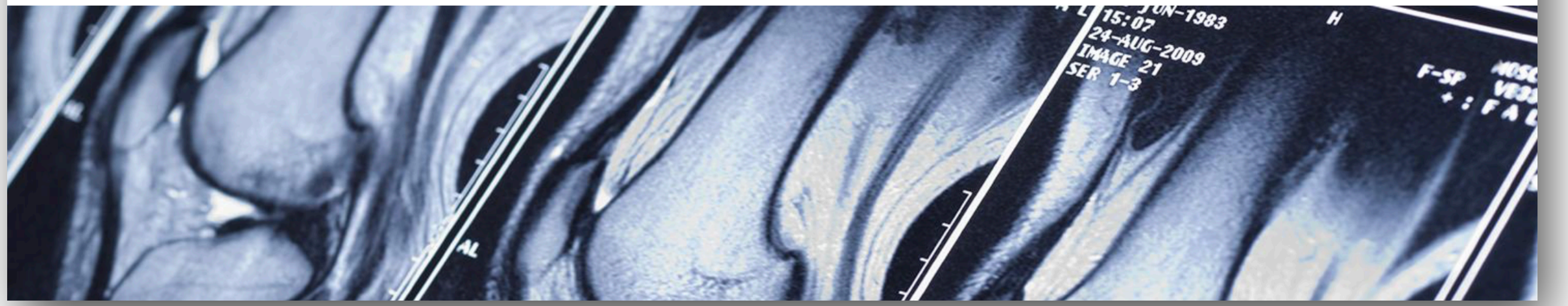

Why do **neural networks** work so well?

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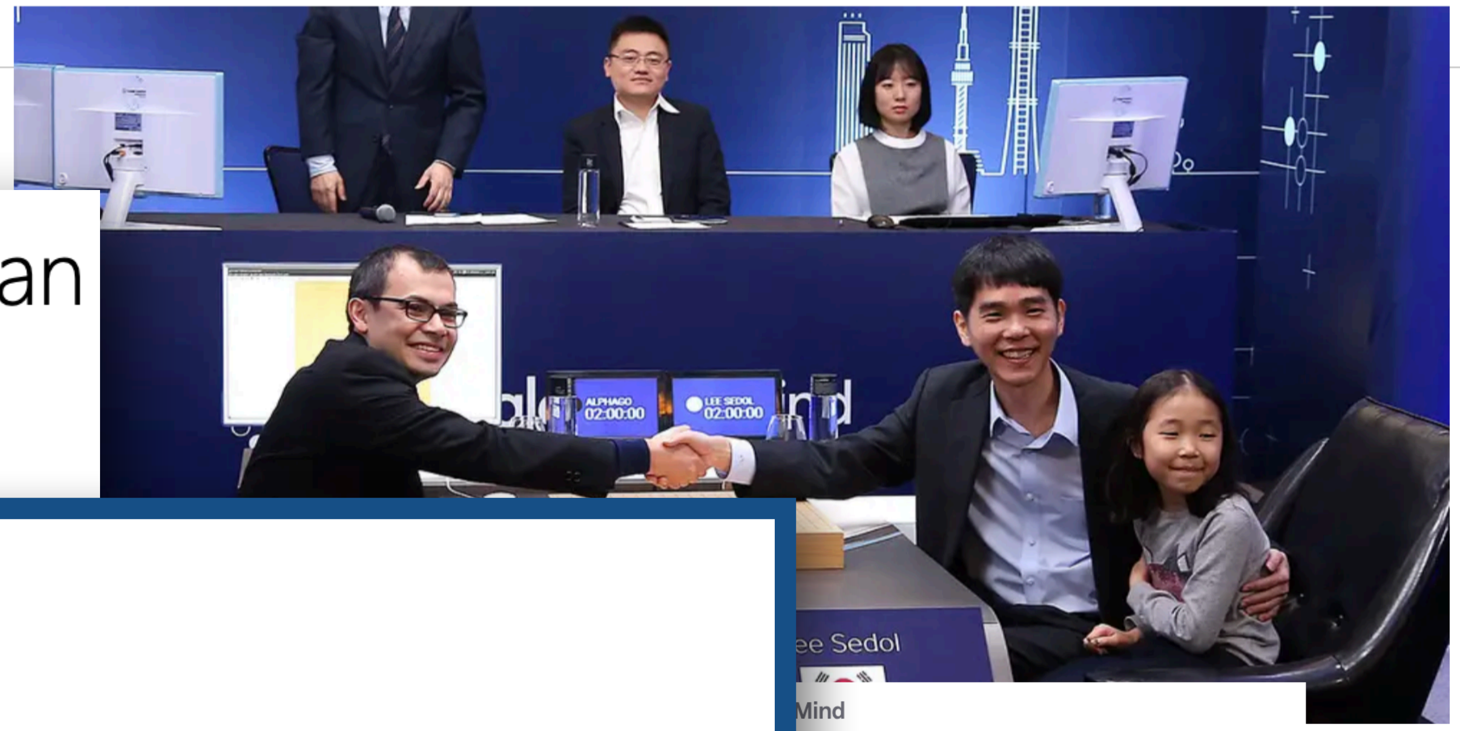

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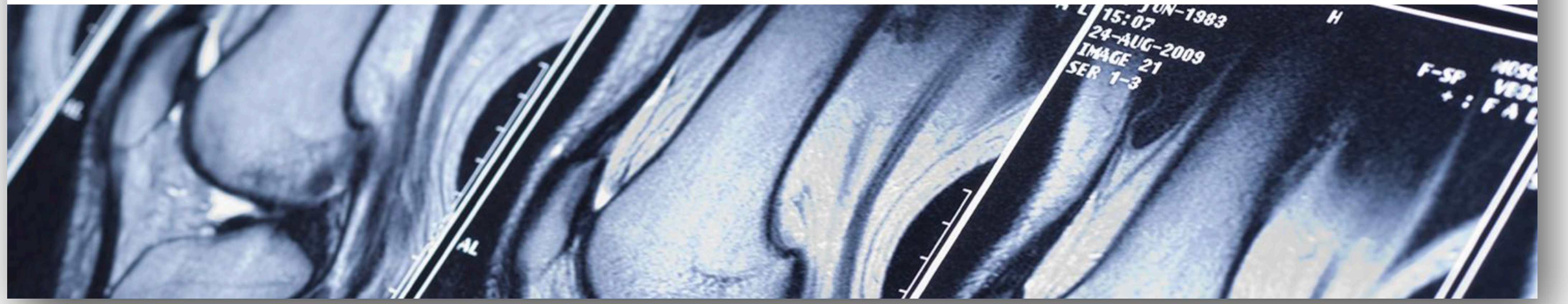

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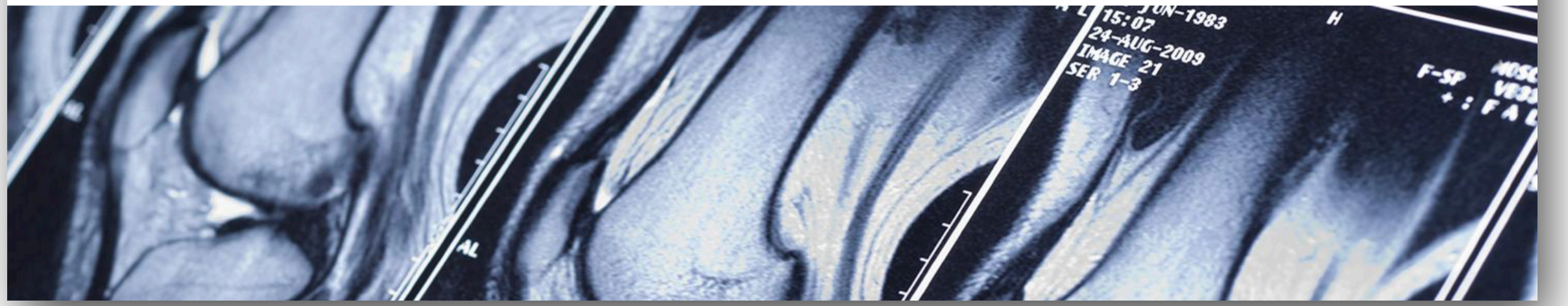

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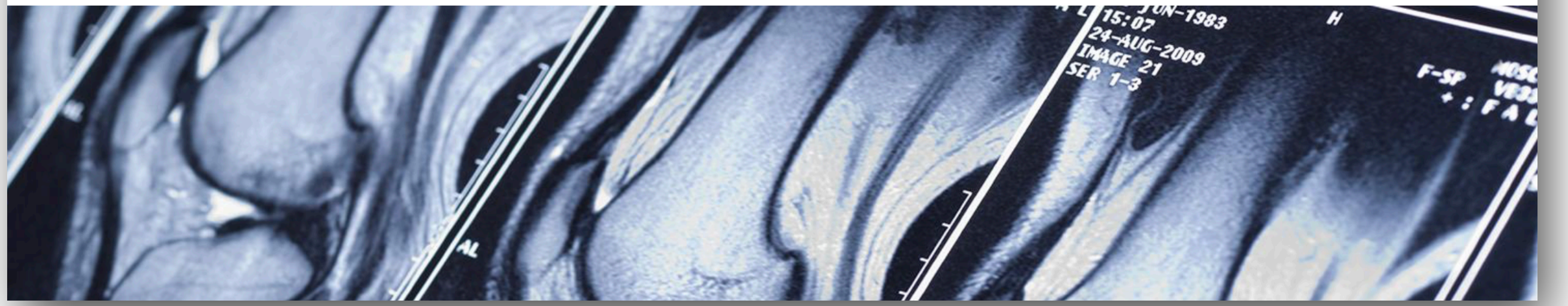
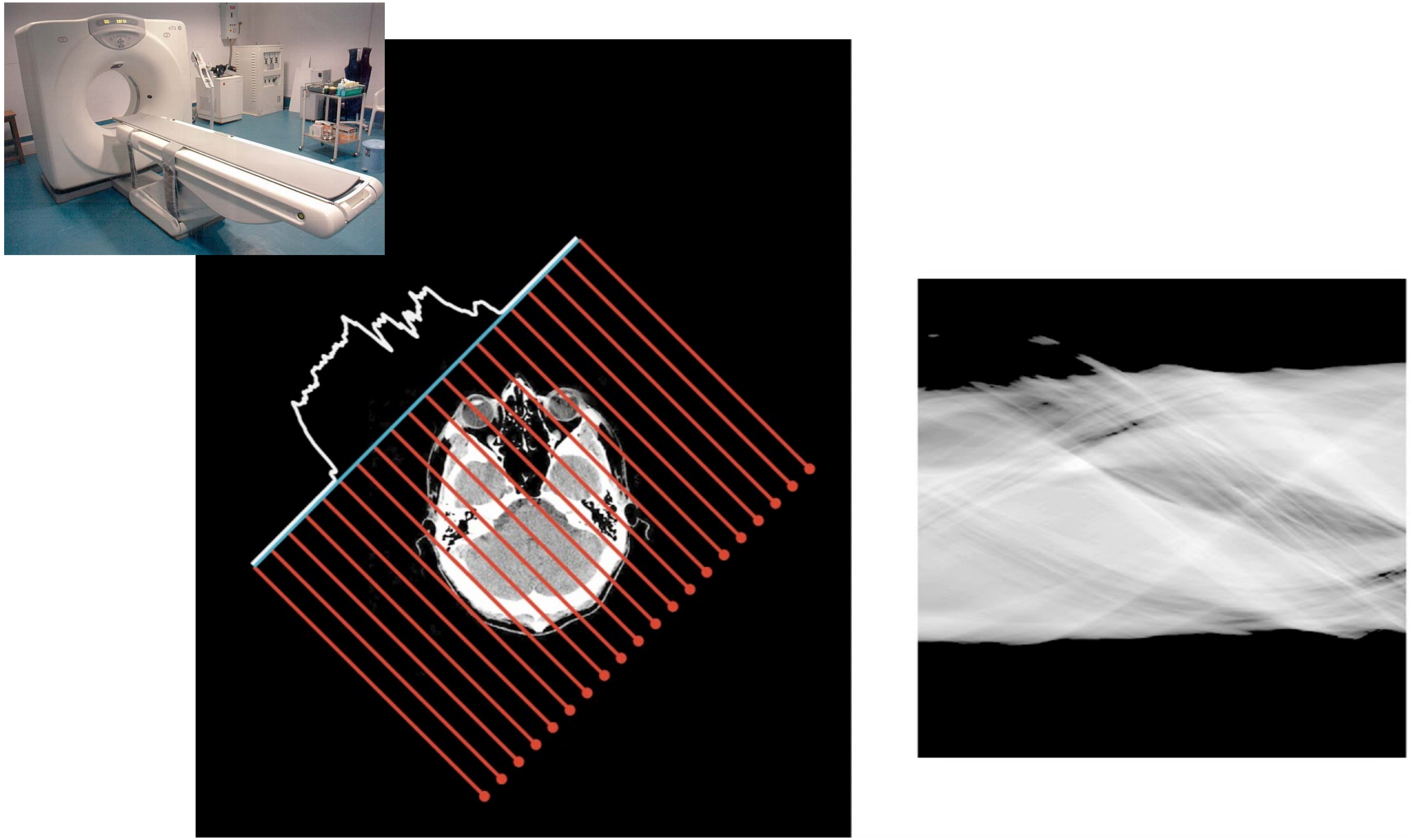


What is an **inverse problem**?

Video from Samuli Siltanen https://www.youtube.com/watch?v=q7Rt_OY_7tU
CT Scan from Andrew Ciscel

What is an **inverse problem**?



Computed Tomography (CT) Scan

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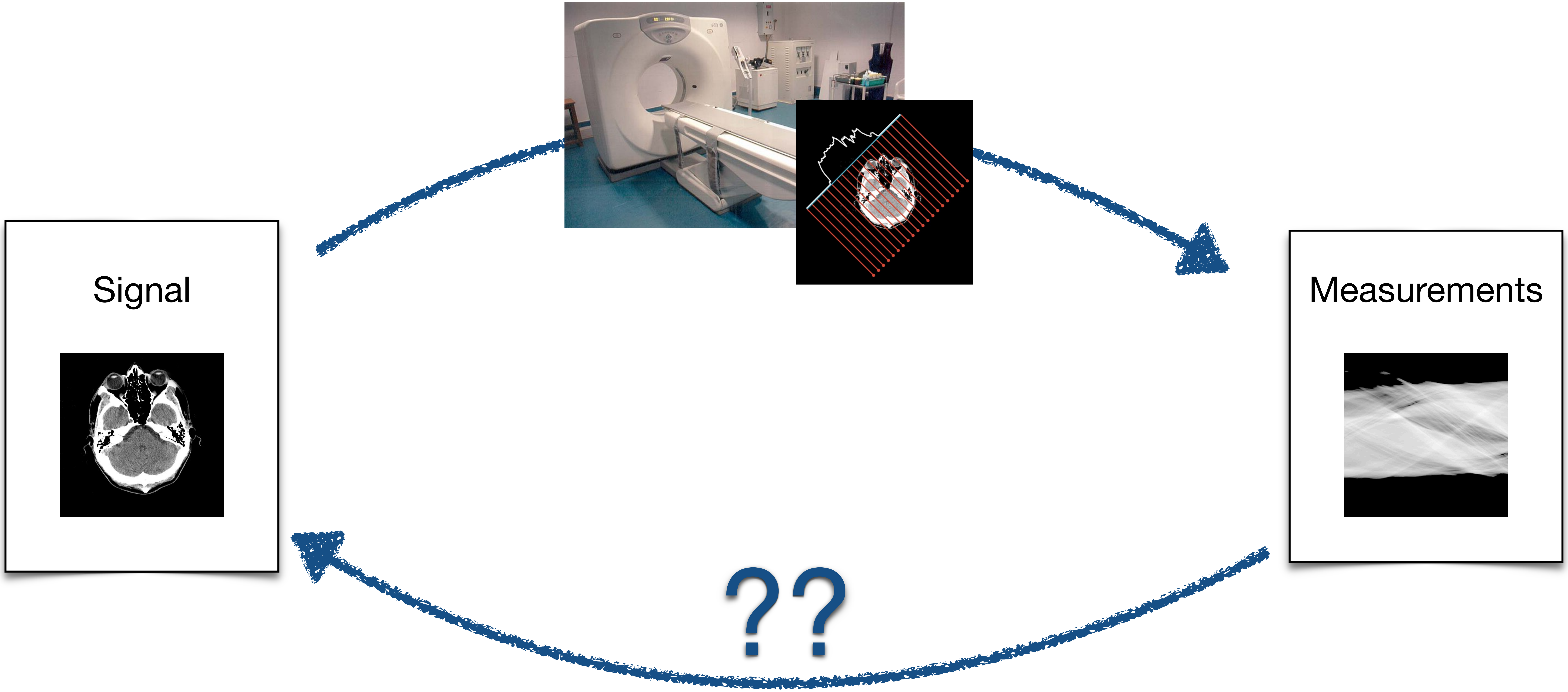
What is an **inverse problem**?



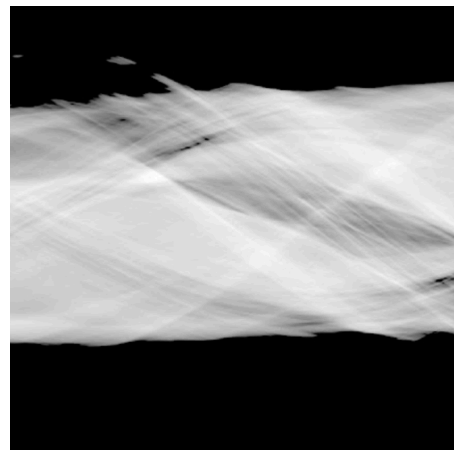
Video from Samuli Siltanen https://www.youtube.com/watch?v=q7Rt_OY_7tU
CT Scan from Andrew Ciscel

What is an **inverse problem**?

$$\mathbf{y}_i = \mathbf{A}(\mathbf{x}_i) \text{ for } i = 1, \ldots, n$$

n examples of this process

Measurements
$\mathbf{y} \in \mathbb{R}^m$



Measurement Operator
$\mathbf{A} : \mathbb{R}^d \to \mathbb{R}^m$

Signal
$\mathbf{x} \in \mathbb{R}^d$

$$\mathbf{y}_{\text{new}} = \mathbf{A}(\mathbf{x}_{\text{new}}) + \varepsilon$$

Measurement Noise
$\varepsilon \in \mathbb{R}^m$

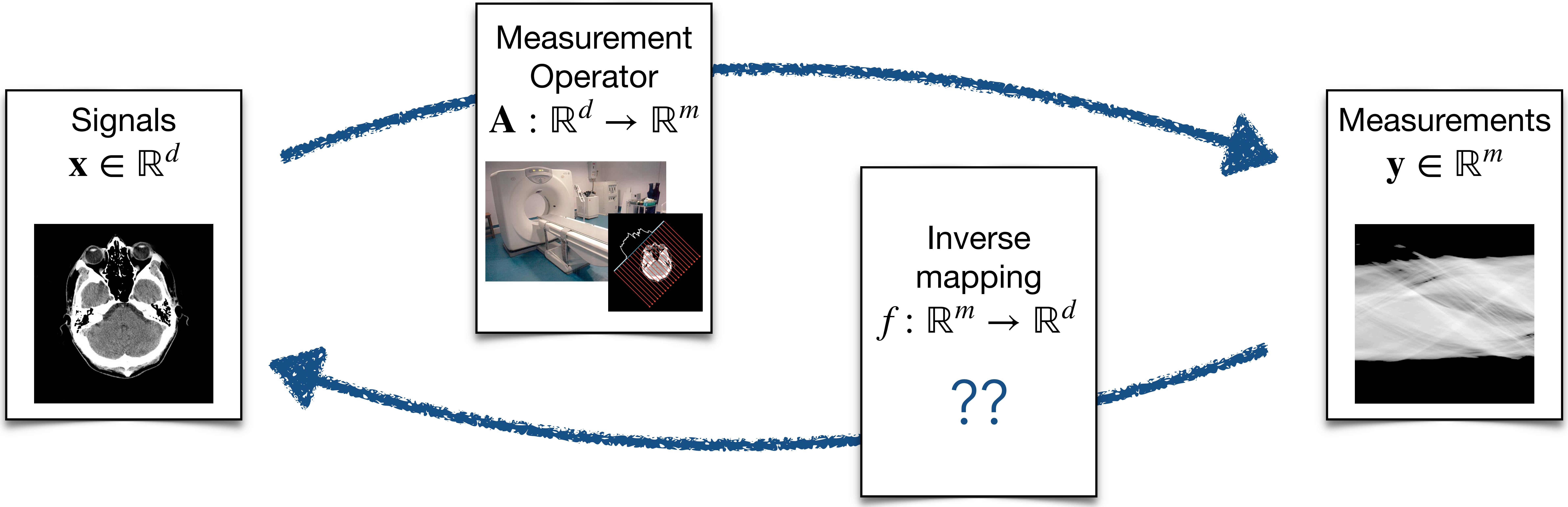
$$m \ll d$$

Given a new observation $\mathbf{y}_{\text{new}}$ our **goal** is to estimate $\mathbf{x}_{\text{new}}$

What is an **inverse problem**?

$$\mathbf{y}_i = \mathbf{A}(\mathbf{x}_i) \text{ for } i = 1, \ldots, n$$

$$\mathbf{y}_{\text{new}} = \mathbf{A}(\mathbf{x}_{\text{new}}) + \varepsilon$$



Given a new observation $\mathbf{y}_{\text{new}}$ our **goal** is to estimate $\mathbf{x}_{\text{new}}$

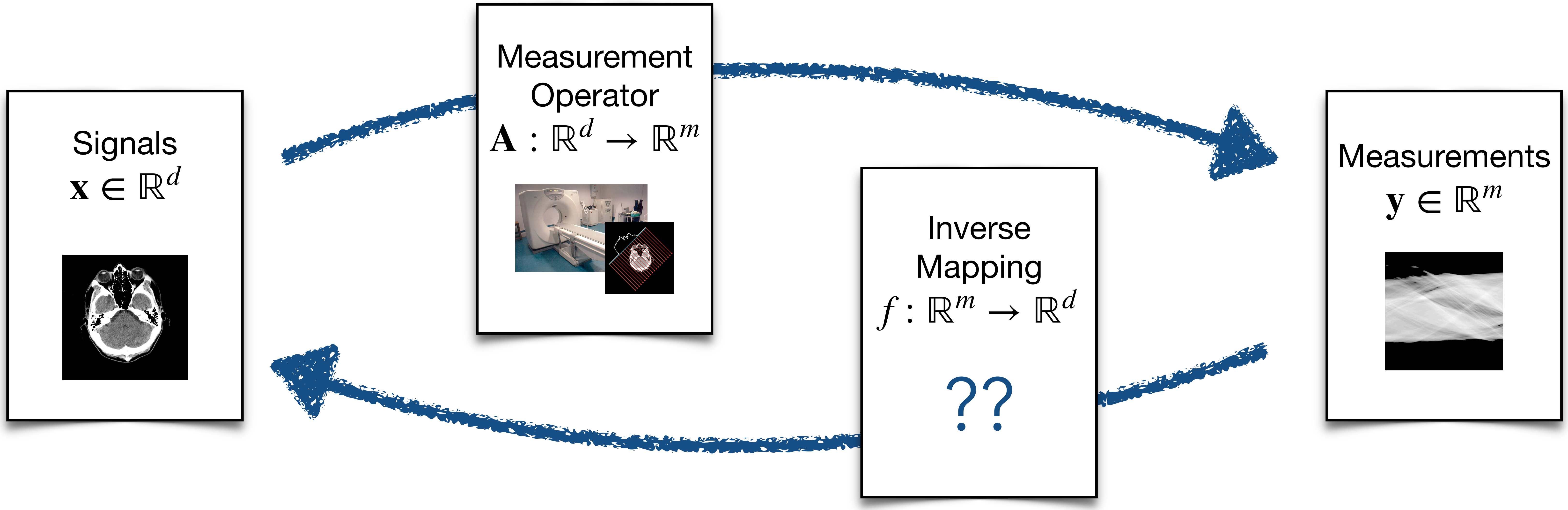
$\iff$

Find a function $f : \mathbf{y}_{\text{new}} \mapsto \mathbf{x}_{\text{new}}$

How did you **traditionally** solve inverse problems?

- Explicitly assume something about the structure of the signal
- Recover the signal as the solution to an optimization problem, regularized according to structural assumptions:

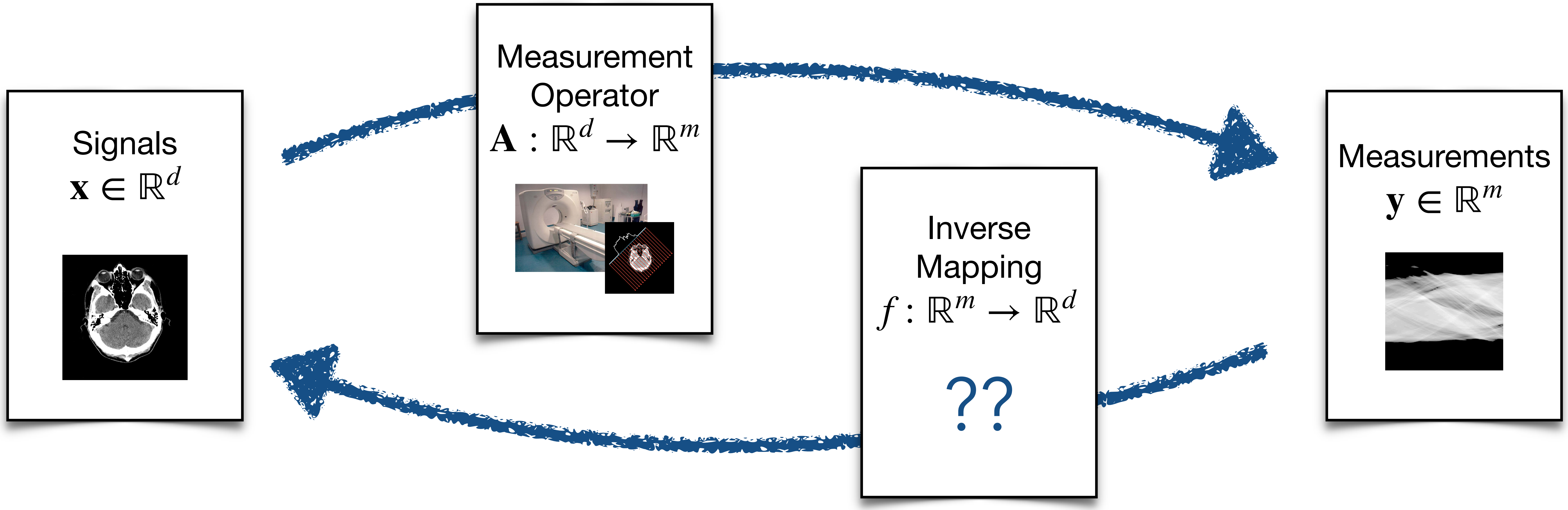
$$\mathbf{x}_{\text{new}} = f(\mathbf{y}_{\text{new}}) = \arg\min_{\mathbf{x}} \|\mathbf{y}_{\text{new}} - \mathbf{A}(\mathbf{x})\|_2^2 + \lambda \|\mathbf{x}\|_2^2$$



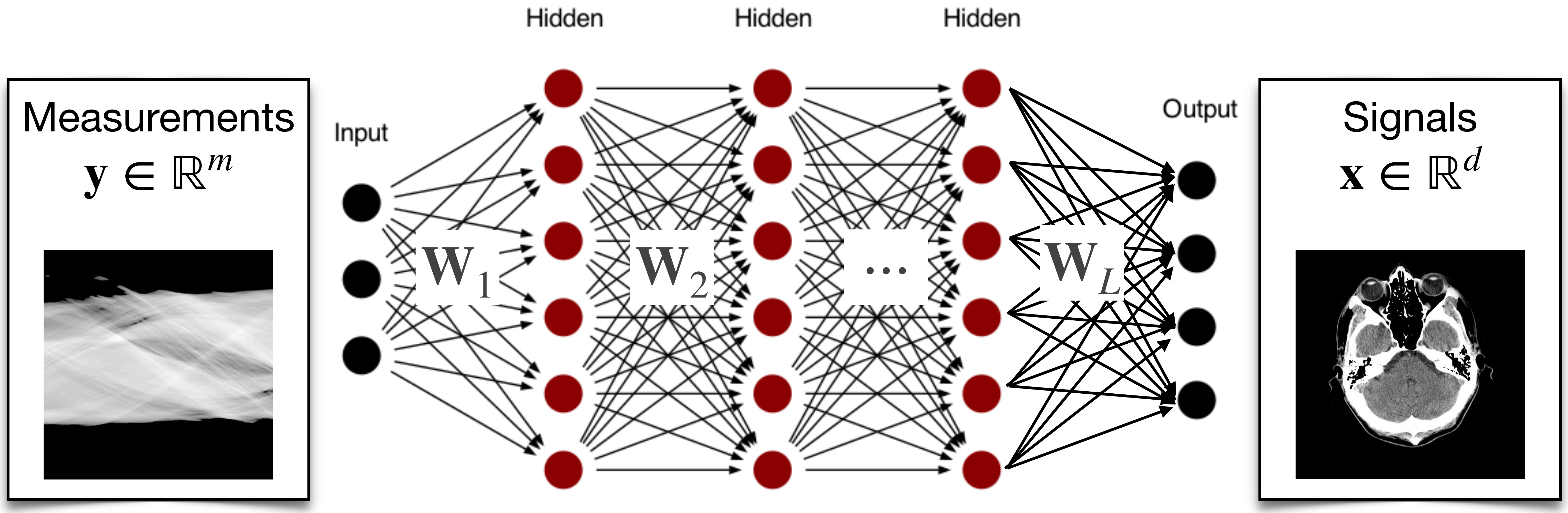
What are **machine learning** approaches to solving an inverse problem?

- If we have access to n training data pairs $\mathbf{y}_i = \mathbf{A}(\mathbf{x}_i)$, can we learn an even better mapping $f : \mathbf{y} \mapsto \mathbf{x}$?
- Pick f in some model class $\mathcal{F}$ that best fits the training data, perhaps plus some regularization

$$\hat{f} = \arg\min_{f \in \mathcal{F}} \; L(f) = \frac{1}{n} \sum_{i=1}^{n} \|f(\mathbf{y}_i) - \mathbf{x}_i\|^2 + R(f)$$



How do you solve inverse problems with a **neural network**?



$$\theta = \left(\mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_L\right)$$

$$f_\theta(\mathbf{y}) = \mathbf{W}_L \sigma\left(\cdots \sigma\left(\mathbf{W}_2 \sigma\left(\mathbf{W}_1 \mathbf{y}\right)\right)\right)$$

Find $\hat{\theta} \in \underset{\theta}{\arg\min} \; L(\theta) = \frac{1}{2} \sum_{i=1}^{n} \|f_\theta(\mathbf{y}_i) - \mathbf{x}_i\|^2 + \lambda \sum_{\ell=1}^{L} \|\mathbf{W}_\ell\|_F^2$

via **Gradient Descent:** $\theta^{t+1} = \theta^t - \eta \nabla L(\theta^t)$

How do you solve inverse problems with a **neural network**?

- Machine learning approaches have been surprisingly successful for solving inverse problems
  Ongie et al. (2018), Barbastathis et al. (2019), Knoll et al (2020)

- The success is especially surprising in light of the very high dimensionality of the data

> Why do **neural networks** work so well for solving **inverse problems**?

- Hypothesis: The training signals have **latent low-dimensional structure** that is preserved by the measurement operator, and neural networks are **adapting to that structure**, allowing for improved robustness to noise at test time. **How does this happen?**

Simplified Setting

- Let us assume that the training signals have a simple form of **latent low-dimensional structure** that is preserved by the measurement operator

- Does a simple neural network **adapt** to that structure? Does this improve **robustness**?

Low-dimensional structure that is **preserved** by the measurement operator

$\mathbf{x}_i = \mathbf{R}\mathbf{z}_i \in \mathbb{R}^d$ and $\mathbf{y}_i = \mathbf{A}\mathbf{x}_i = \mathbf{A}\mathbf{R}\mathbf{z}_i \in \mathbb{R}^m$

$n \geq s$ samples of this process

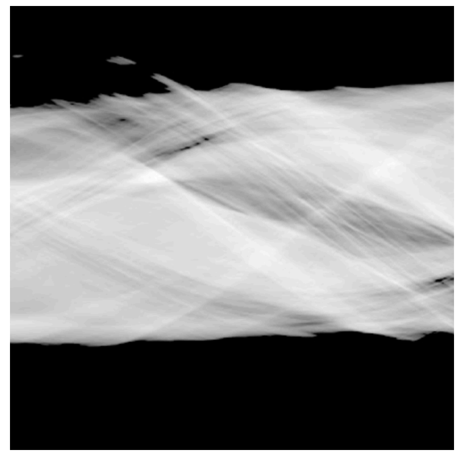
$\mathbf{R} \in \mathbb{R}^{d \times s}$

Signals live in an s-dimensional subspace $\mathbf{x} \in \text{range}(\mathbf{R}) \subseteq \mathbb{R}^d$

Linear measurement operator $\mathbf{A} \in \mathbb{R}^{m \times d}$ preserves the subspace structure

$(1-\delta)\|\mathbf{x}\| \leq \|\mathbf{A}\mathbf{x}\| \leq (1+\delta)\|\mathbf{x}\|$ $\forall \mathbf{x} \in \text{range}(\mathbf{R})$

Measurements live in an s-dimensional subspace $\mathbf{y} \in \text{range}(\mathbf{A}\mathbf{R}) \subseteq \mathbb{R}^m$



$$s \ll m \ll d$$

$$\mathbf{y}_{\text{new}} = \mathbf{A}\mathbf{x}_{\text{new}} + \varepsilon = \mathbf{A}\mathbf{R}\mathbf{z}_{\text{new}} + \varepsilon$$

Measurement Noise $\varepsilon \in \mathbb{R}^m$

Warning: What follows is **not** advice on how to solve this inverse problem!

- If you know *a priori* that your inverse problem has this subspace structure, then there is a known way recover $\mathbf{x}_{\text{new}}$ with high accuracy
- **Oracle solution** using the Moore-Penrose Pseudoinverse:

Stack n samples into matrices $\mathbf{X} \in \mathbb{R}^{d \times n}$ and $\mathbf{Y} \in \mathbb{R}^{m \times n}$

$$\mathbf{x}_{\text{new}} \approx \mathbf{R}(\mathbf{A}\mathbf{R})^{\dagger}\mathbf{y}_{\text{new}} = \mathbf{X}\mathbf{Y}^{\dagger}\mathbf{y}_{\text{new}}$$

- Precisely because the oracle solution exists, we can analyze how close the learned neural network is to doing the "right" thing
- An inverse mapping that takes advantage of the **low-dimensional structure** does much better than one that does not
- What does this simplified setting reveal about the ability of neural networks to **automatically adapt to structure** in data?

$$\mathbf{x}_i = \mathbf{R}\mathbf{z}_i \in \mathbb{R}^d \text{ and } \mathbf{y}_i = \mathbf{A}\mathbf{x}_i = \mathbf{A}\mathbf{R}\mathbf{z}_i \in \mathbb{R}^m$$

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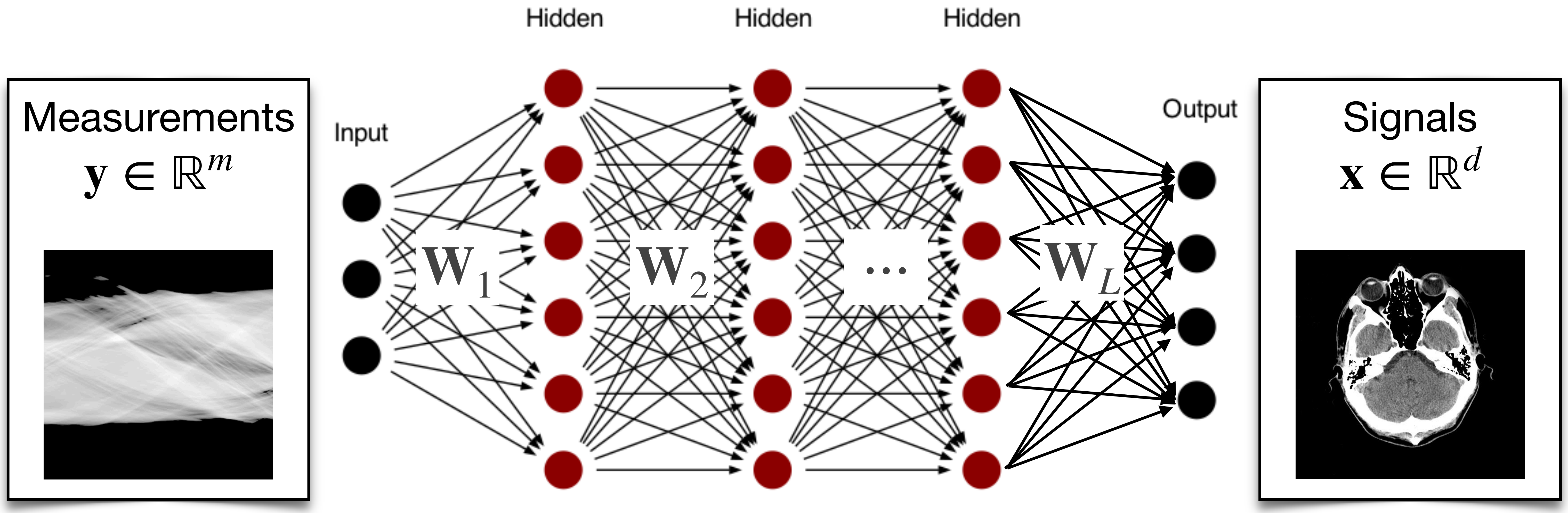
Neural Network with Linear Activations



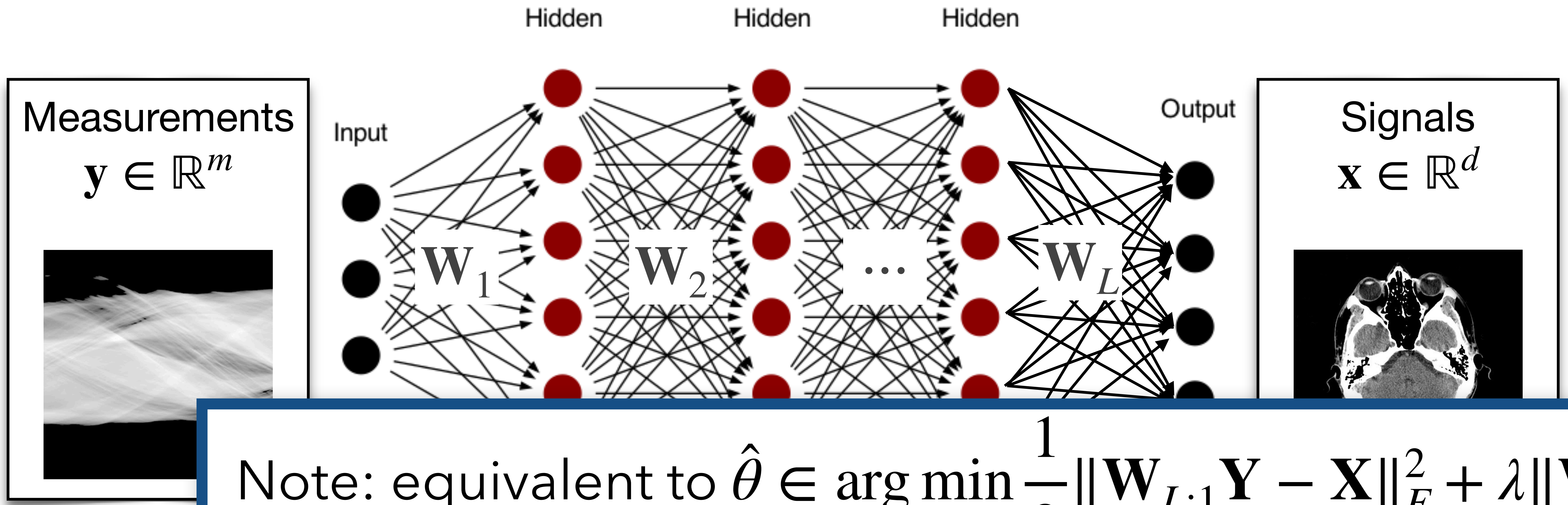
$$\theta = \left(\mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_L\right)$$

$$f_\theta(\mathbf{y}) = \mathbf{W}_L \cdots \mathbf{W}_2 \mathbf{W}_1 \mathbf{y}$$

Find $\hat{\theta} \in \arg\min_{\theta} \; L(\theta) = \frac{1}{2}\|\mathbf{W}_L \cdots \mathbf{W}_1 \mathbf{Y} - \mathbf{X}\|_F^2 + \lambda \sum_{\ell=1}^{L} \|\mathbf{W}_\ell\|_F^2$

via **Gradient Descent:** $\theta^{t+1} = \theta^t - \eta \nabla L(\theta^t)$

Neural Network with Linear Activations



Never explicitly imposing low-dimensional structure!

$$\theta = \left(\mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_L\right)$$

$$f_\theta(\mathbf{y}) = \mathbf{W}_L \cdots \mathbf{W}_2 \mathbf{W}_1 \mathbf{y}$$

Note: equivalent to $\hat{\theta} \in \arg\min_{\theta} \frac{1}{2} \|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F^2 + \lambda \|\mathbf{W}_{L:1}\|_{S^{2/L}}^{2/L}$

But gradient descent trajectory may be different!

Find $\hat{\theta} \in \arg\min_{\theta} \; L(\theta) = \frac{1}{2} \|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F^2 + \lambda \sum_{\ell=1}^{L} \|\mathbf{W}_\ell\|_F^2$

via **Gradient Descent:** $\theta^{t+1} = \theta^t - \eta \nabla L(\theta^t)$

Previous work on gradient descent in linear neural networks

- Without regularization ($\lambda = 0$) *Du & Hu (2019), Xu et al. (2023)*
- Unrealistic initialization assumptions *Hu et al. (2020), Hu et al. (2022), Arora et al. (2019), Nguegnang et al. (2024), Arora et al. (2018)*
- Step-size η very small *Lewkowycz & Gur-Ari (2020), Gidel et al. (2019), Ji & Telgarsky (2019), Eftekhari (2020), Bah et al. (2019), Pesme et al. (2021), Jacot et al. (2021), Arora et al. (2018),*
- SGD can only ever decrease the rank of a solution, but unclear if it finds a good fit to the data *Wang & Jacot (2024)*

Our analysis

➡With regulariation ($\lambda > 0$)

➡Initialization essentially equivalent to using **PyTorch default**

➡Very **mild** assumptions on stepsize η

➡**Both** adaptation to structure and good fit to the training data

So **what happens** in our simplified setting?

$\mathbf{x}_i = \mathbf{R}\mathbf{z}_i \in \mathbb{R}^d$ and $\mathbf{y}_i = \mathbf{A}\mathbf{x}_i = \mathbf{A}\mathbf{R}\mathbf{z}_i \in \mathbb{R}^m$

$\mathbf{y}_{\text{new}} = \mathbf{A}\mathbf{x}_{\text{new}} + \varepsilon = \mathbf{A}\mathbf{R}\mathbf{z}_{\text{new}} + \varepsilon$

Find $\hat{\theta} \in \arg\min_{\theta} \; L(\theta) = \frac{1}{2}\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F^2 + \lambda \sum_{\ell=1}^{L} \|\mathbf{W}_\ell\|_F^2$

via **Gradient Descent:** $\theta^{t+1} = \theta^t - \eta \nabla L(\theta^t)$

We track the evolution of **two main quantities** throughout gradient descent:

$\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F$ and $\|\mathbf{W}_{L:1}\mathbf{P}_\perp\|_2$

How well network reconstructs the training data

How well network adapts to low-dimensional structure

$\mathbf{P}_\perp$ = projection onto range$(\mathbf{A}\mathbf{R})^\perp$

Good reconstructions of training data & adaptation to structure
$\Longrightarrow$ robustness to noise at test-time

$$\|\mathbf{W}_{L:1}\mathbf{y}_{\text{new}} - \mathbf{x}_{\text{new}}\|_2 \leq \|\mathbf{W}_{L:1} - \mathbf{X}\mathbf{Y}^\dagger\|_2 \|\mathbf{y}_{\text{new}}\|_2 + \|\mathbf{X}\mathbf{Y}^\dagger\mathbf{y}_{\text{new}} - \mathbf{x}_{\text{new}}\|_2$$

$$\|\mathbf{W}_{L:1} - \mathbf{X}\mathbf{Y}^\dagger\|_2 \leq \|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F \|\mathbf{Y}^\dagger\|_2 + \|\mathbf{W}_{L:1}\mathbf{P}_\perp\|_2$$

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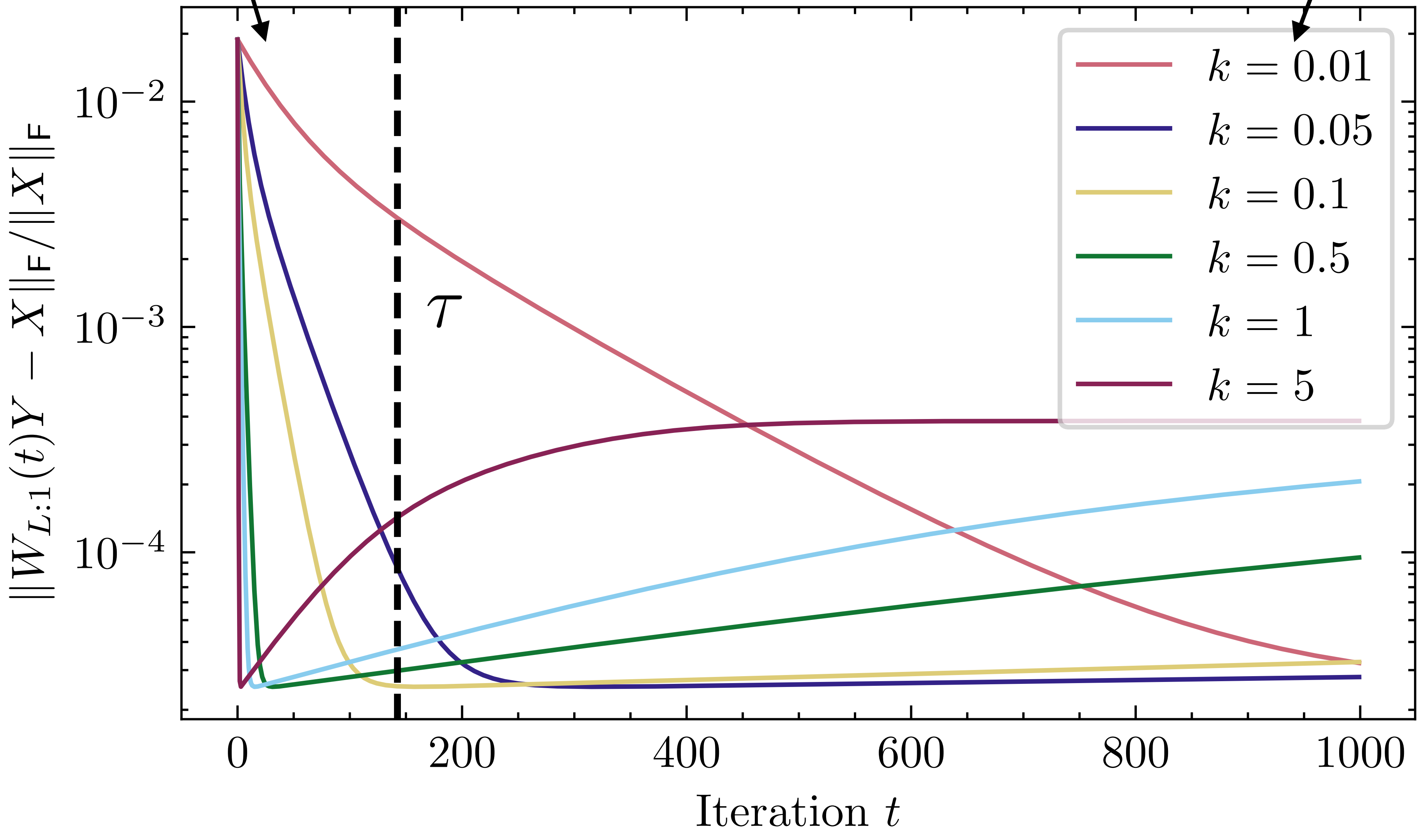
How well network reconstructs the training data

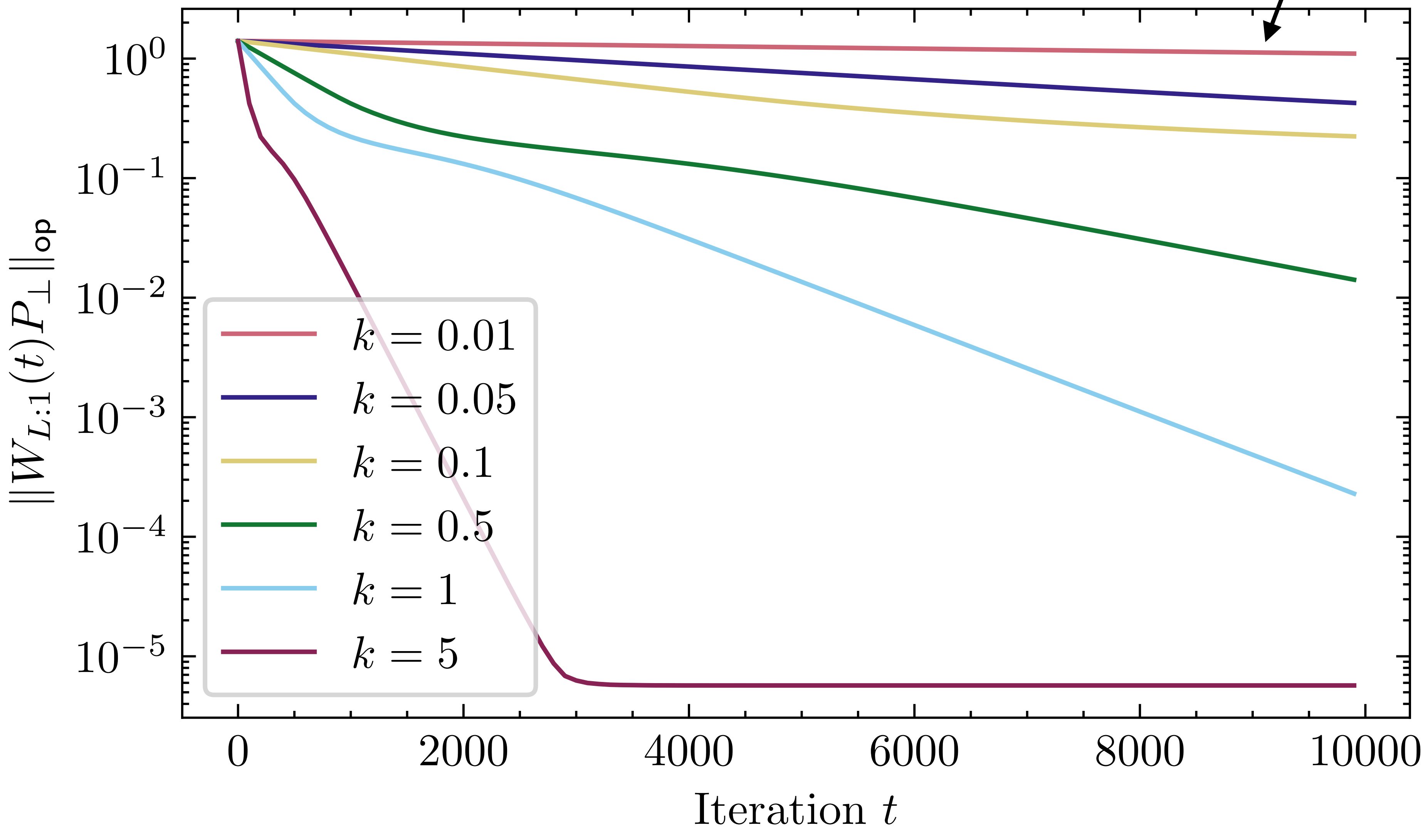
$\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F$

Training with different stepsizes $\eta = k \cdot \hat{\eta}$ where $\hat{\eta}$ is the stepsize prescribed by our theory



$\|\mathbf{W}_{L:1}\mathbf{P}_\perp\|_2$

How well network adapts to low-dimensional structure



Two phases:

1. **Rapid** improvement in **reconstructions** of the training samples in first τ iterations
2. **Slow** recovery of the latent low-dimensional **structure**

So **what happens** in our simplified setting?

$$\mathbf{x}_i = \mathbf{R}\mathbf{z}_i \in \mathbb{R}^d \text{ and } \mathbf{y}_i = \mathbf{A}\mathbf{x}_i = \mathbf{A}\mathbf{R}\mathbf{z}_i \in \mathbb{R}^m$$

$$\mathbf{y}_{\text{new}} = \mathbf{A}\mathbf{x}_{\text{new}} + \varepsilon = \mathbf{A}\mathbf{R}\mathbf{z}_{\text{new}} + \varepsilon$$

$$\text{Find } \hat{\theta} \in \arg\min_{\theta} \; L(\theta) = \frac{1}{2}\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F^2 + \lambda \sum_{\ell=1}^{L} \|\mathbf{W}_\ell\|_F^2$$

via **Gradient Descent:** $\theta^{t+1} = \theta^t - \eta \nabla L(\theta^t)$

Two phases:

1. **Rapid** improvement in reconstructions of the **training** samples

$$\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F = O\left(\frac{\lambda}{L}\right)$$

after $\tau = O\left(\frac{1}{\eta L}\log\left(\frac{L}{\lambda}\right)\right)$ iterations

2. **Slow** recovery of the latent low-dimensional **structure**

$$\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F = O(\lambda) \text{ and } \|\mathbf{W}_{L:1}\mathbf{P}_\perp\|_2 = O\left(\frac{1}{d_w^C}\right)$$

after $T = O\left(\frac{\log(d_w)}{\eta\lambda}\right)$ iterations

Good reconstructions of training data & adaptation to structure

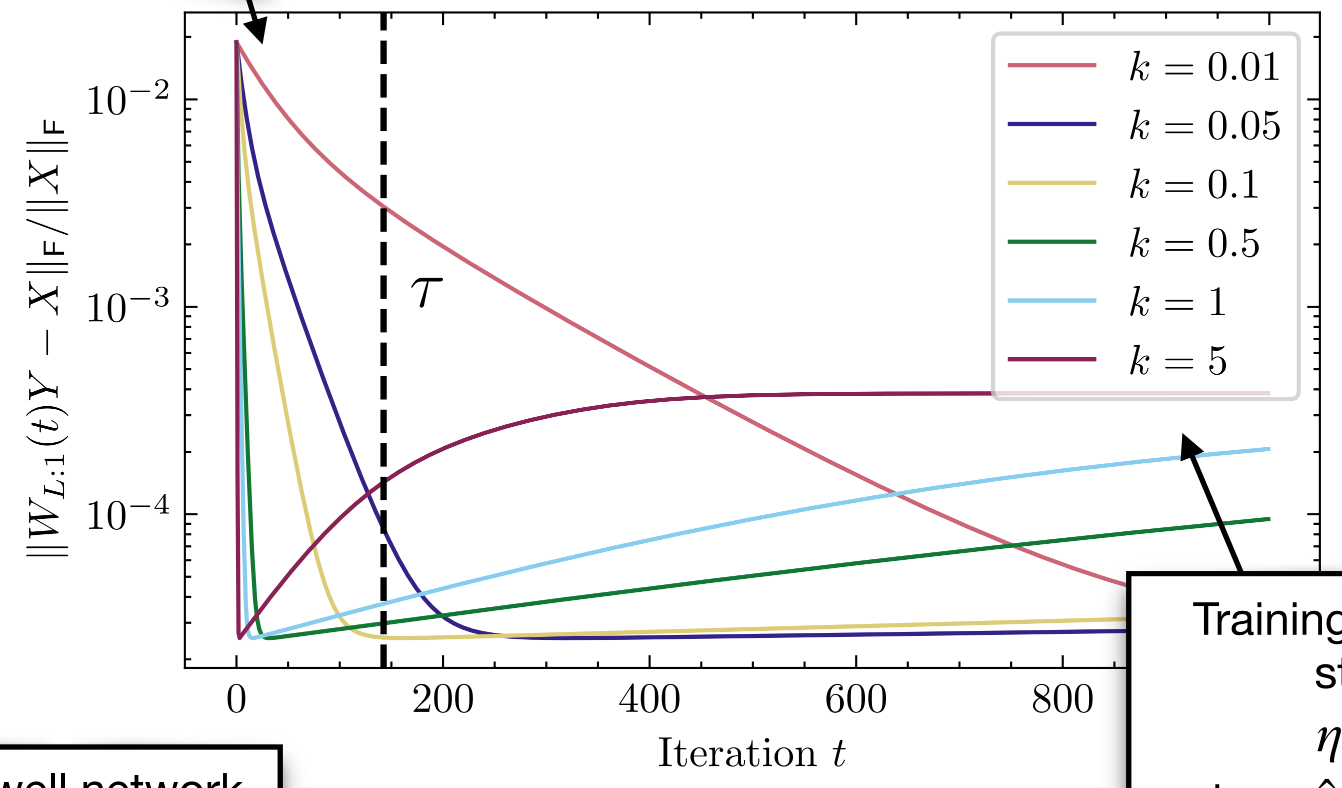
$\Longrightarrow$ robustness to noise at test-time

$$\|\mathbf{W}_{L:1} - \mathbf{X}\mathbf{Y}^\dagger\|_2 \le \|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F \|\mathbf{Y}^\dagger\|_2 + \|\mathbf{W}_{L:1}\mathbf{P}_\perp\|_2$$

Distance to **oracle** solution is small at the end of Phase 2

How well network reconstructs the training data

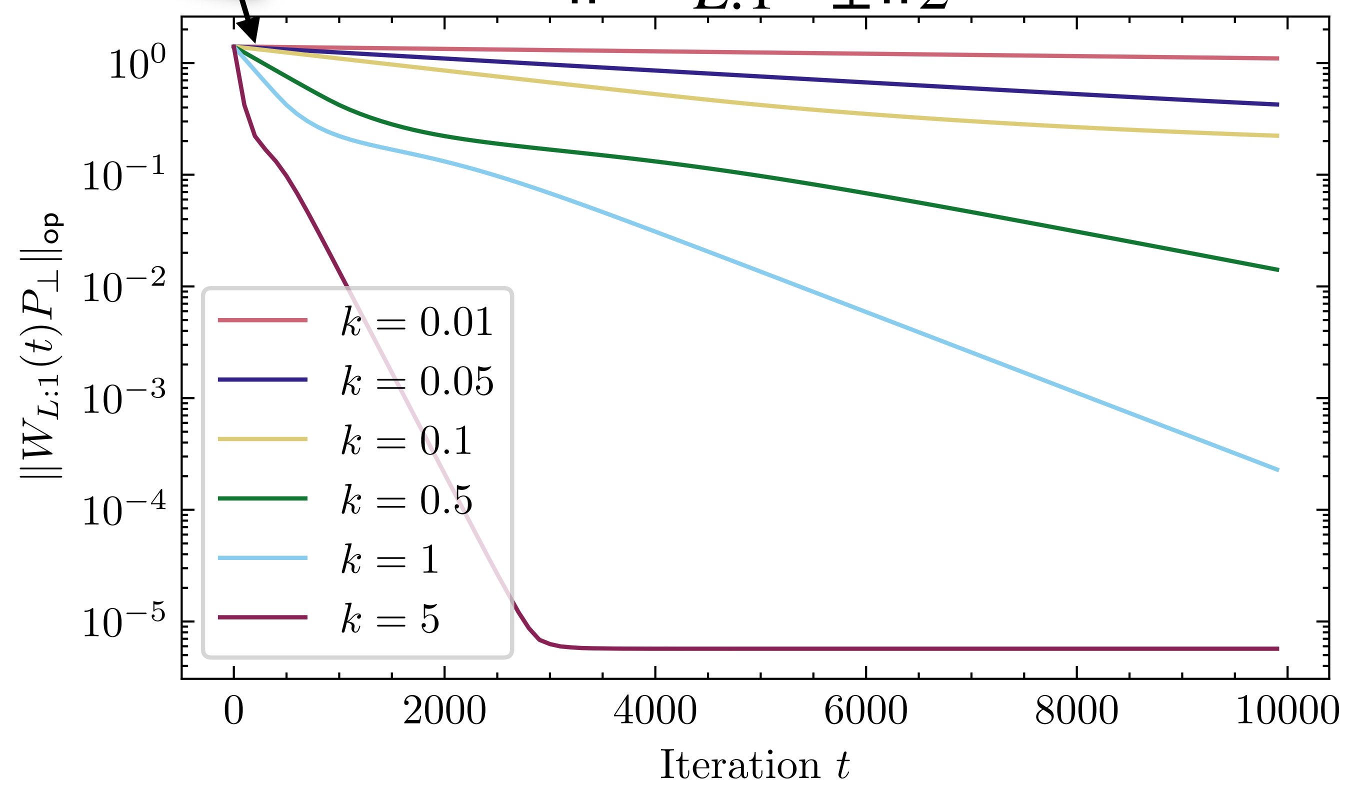
$\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F$



Training with different stepsizes $\eta = k \cdot \hat{\eta}$ where $\hat{\eta}$ is the stepsize prescribed by our theory

How well network adapts to low-dimensional structure

$\|\mathbf{W}_{L:1}\mathbf{P}_\perp\|_2$



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$\mathbf{y}_{\text{new}} = \mathbf{A}\mathbf{x}_{\text{new}} + \varepsilon = \mathbf{A}\mathbf{R}\mathbf{z}_{\text{new}} + \varepsilon$

Find $\hat{\theta} \in \arg\min_{\theta} \; L(\theta) = \frac{1}{2}\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F^2 + \lambda \sum_{\ell=1}^{L} \|\mathbf{W}_\ell\|_F^2$

via **Gradient Descent:** $\theta^{t+1} = \theta^t - \eta \nabla L(\theta^t)$

Two phases:

1. **Rapid** improvement in reconstructions of the **training** samples

$$\|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F = O\left(\frac{\lambda}{L}\right)$$

afte

2. **Slow** recovery of the la

$\|\mathbf{W}_{L:1}\mathbf{Y} -$

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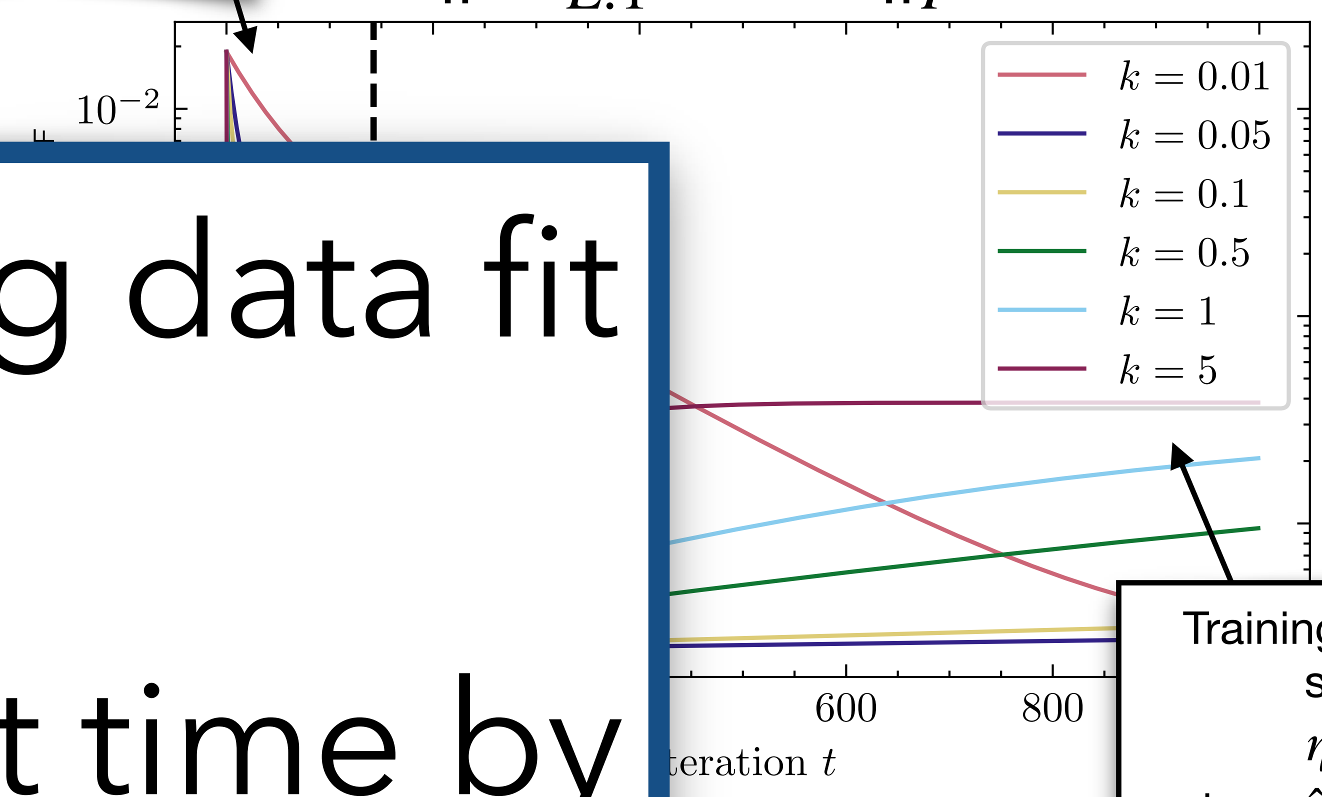
Continuing to train after training data fit stops improving →
Network that does better at test time by adapting to low-dimensional structure

How well network reconstructs the training data



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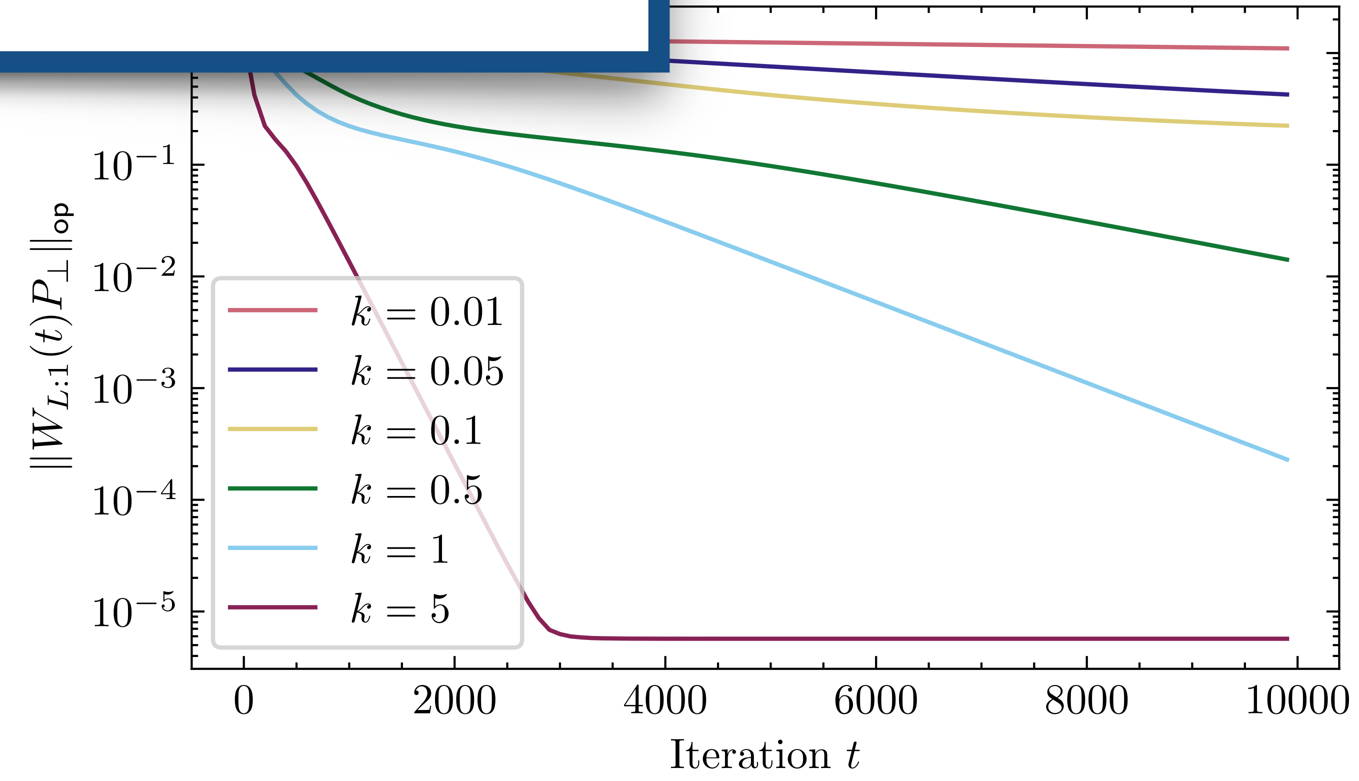


Good reconstructions of training data & adaptation to structure
$\Longrightarrow$ robustness to noise at test-time

$$\|\mathbf{W}_{L:1} - \mathbf{X}\mathbf{Y}^\dagger\|_2 \leq \|\mathbf{W}_{L:1}\mathbf{Y} - \mathbf{X}\|_F \|\mathbf{Y}^\dagger\|_2 + \|\mathbf{W}_{L:1}\mathbf{P}_\perp\|_2$$

Distance to **oracle** solution is small at the end of Phase 2

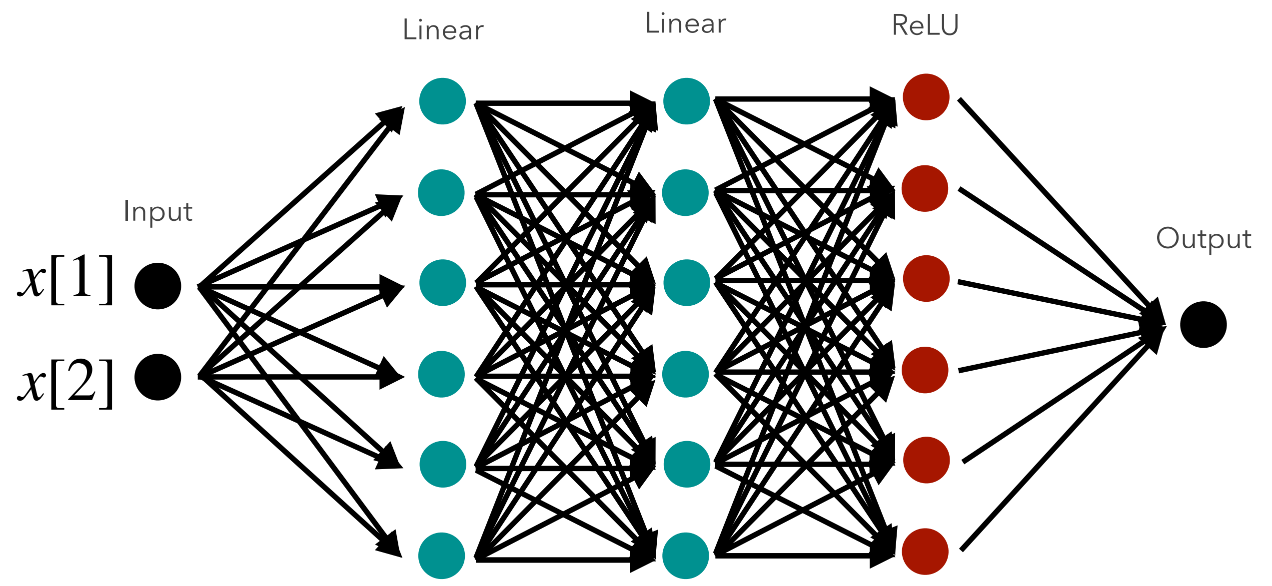
One reason **neural networks** work well for solving **inverse problems** is because they can **automatically adapt** to structure in data

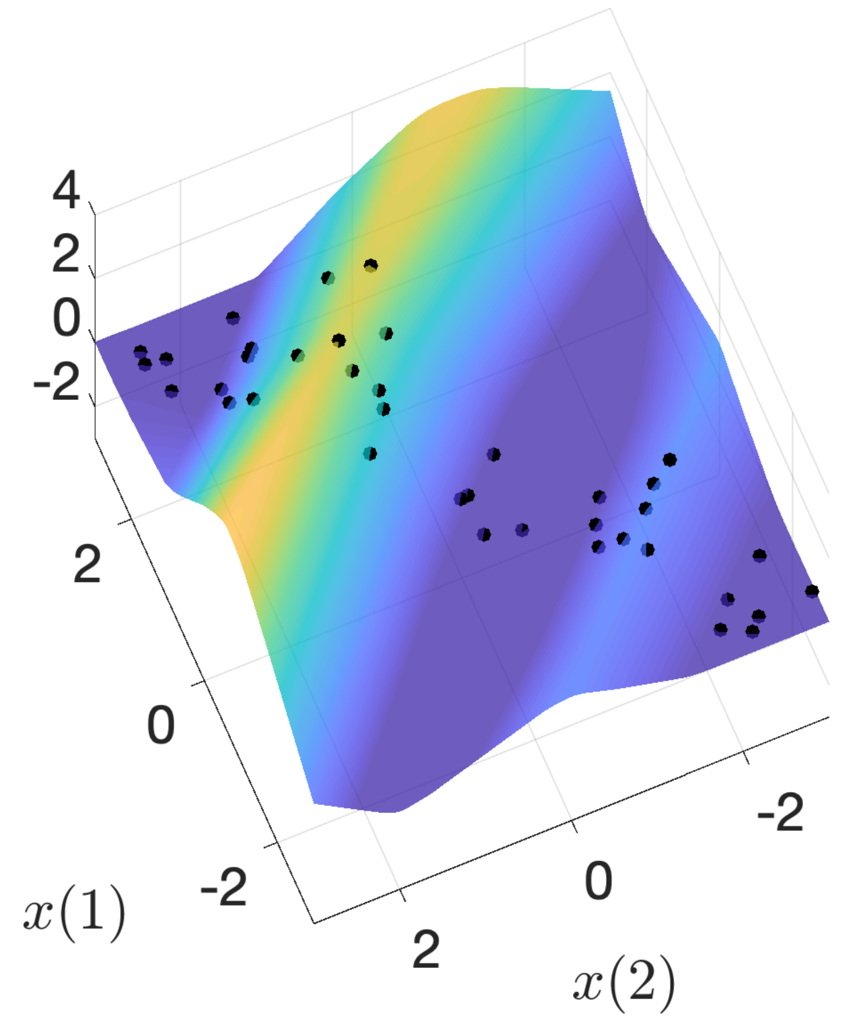
What’s next?

- What about more complex forms of low-dimensional structure in data?
- What about more complex neural networks?
- How does depth affect the ability to adapt to low-dimensional structure?
- What about stochastic variants of gradient descent? Adam, etc.?

What else?

- Studying how nonlinear neural network architectures adapt to low-dimensional structure
  - Adding linear layers to a ReLU network yields a trained network that mostly **only varies in a few directions** in the input space *Parkinson, Ongie & Willett (2025)*
  - Functions that can be represented by a deep ReLU network with small **norm** will have low-dimensional structure *Jacot (2023)*
  - Similar behavior can be induced with only a few ReLU layers and many linear layers
- What can **deeper** networks do that **shallower** networks can't? *Parkinson, Ongie, Willett, Shamir & Srebro (2024)*





Thank you!

https://arxiv.org/abs/2502.15522

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