Maximum Mean Discrepancy Gradient Flow

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Outline

- General problem
- Wasserstein gradient of the MMD
- A Criterion for global convergence
- A noise-injection algorithm for better convergence

General problem

Finite dimensional non-convex optimization:

$$\min_{Z^1,\dots,Z^N \in \mathcal{Z}} \mathcal{L}\left(\frac{1}{N}\sum_{i=1}^{N} \delta_{Z^n}\right)$$

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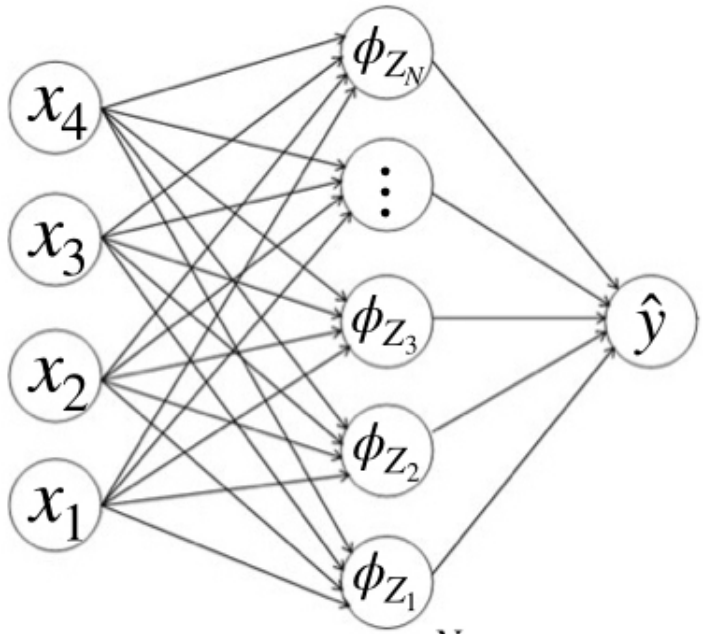
$$(x, y) \sim data$$



$$\min_{Z_1,\dots,Z_N} \mathbb{E}_{data}[\|y - \frac{1}{N}\sum_{i=1}^{N} \phi_{Z_i}(x)\|^2]$$

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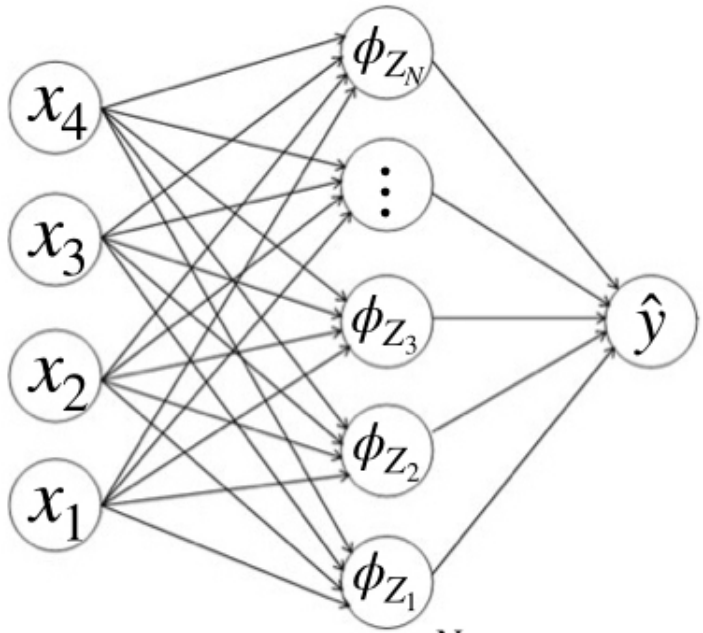

$$\min_{Z_1,\dots,Z_N} \mathbb{E}_{data}[\|y - \frac{1}{N}\sum_{i=1}^{N} \phi_{Z_i}(x)\|^2]$$

- Optimization using gradient descent GD:

$$Z^n_{t+1} = Z^n_t - \gamma \nabla_{Z^n} \mathcal{L}\left(\frac{1}{N}\sum_{i=1}^{N} \delta_{Z^n_t}\right)$$

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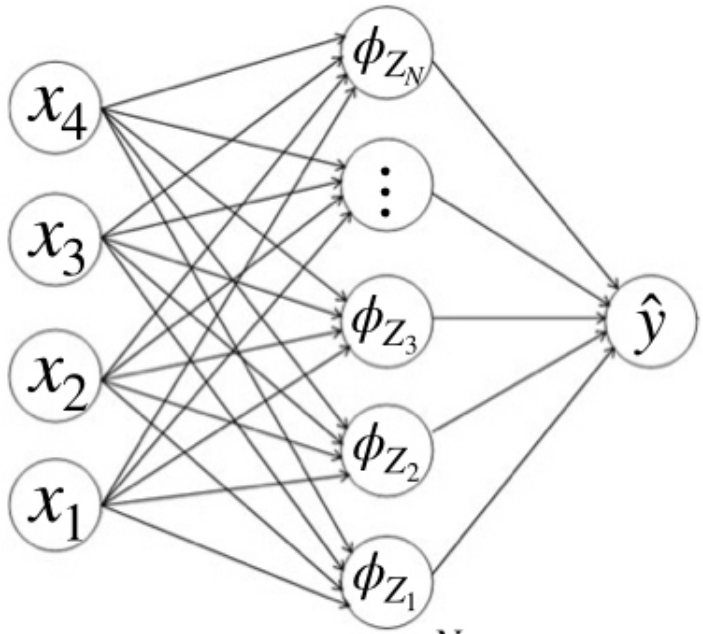

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- Hard to describe the dynamics of GD!

General problem

Infinite dimensional non-convex optimization:

$$\min_{z^1,\dots,z^N \in \mathcal{Z}} \mathcal{L}\left(\frac{1}{N}\sum_{i=1}^{N} \delta_{z^n}\right) \quad \xrightarrow[N\to\infty]{} \quad \min_{\nu \in \mathcal{P}} \mathcal{L}(\nu)$$

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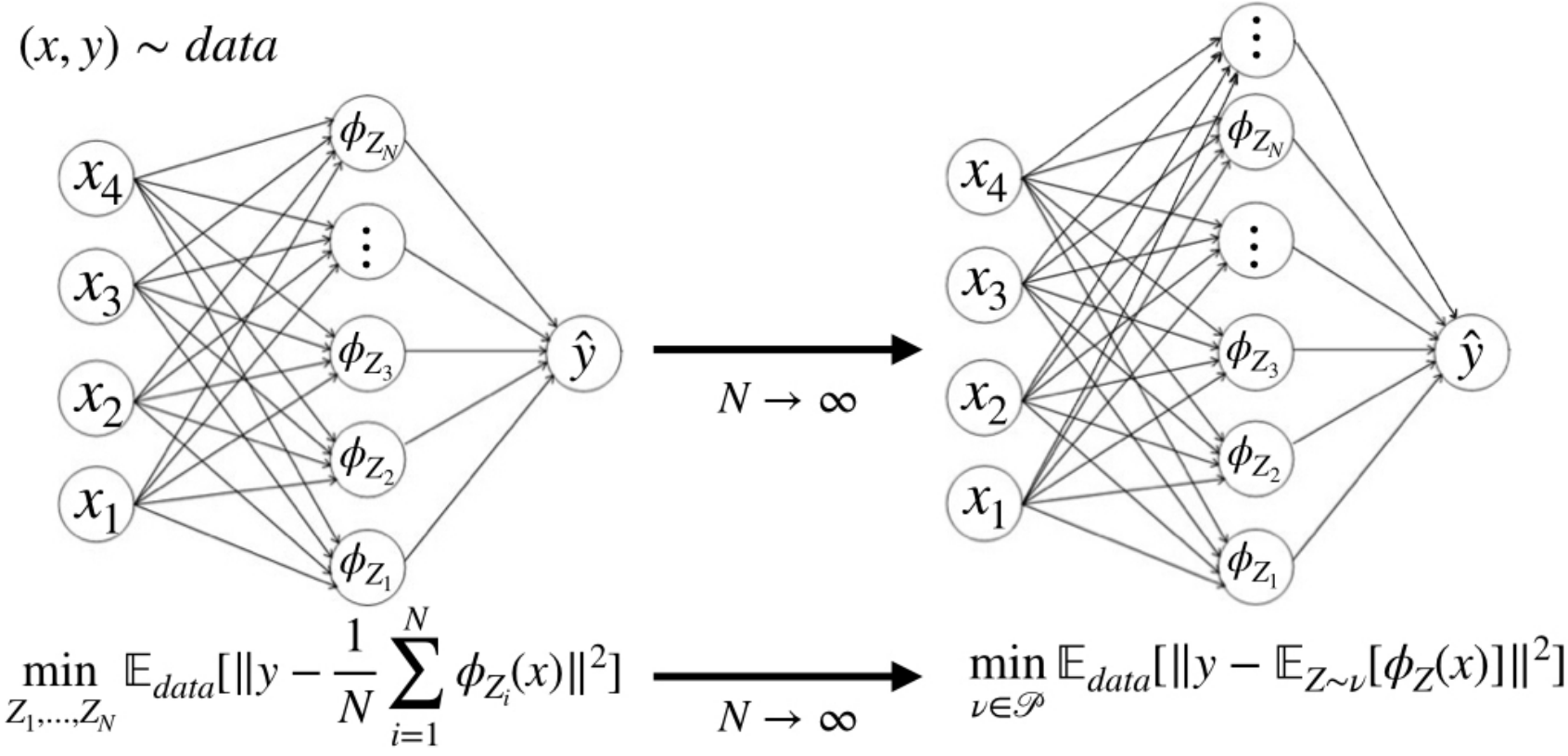
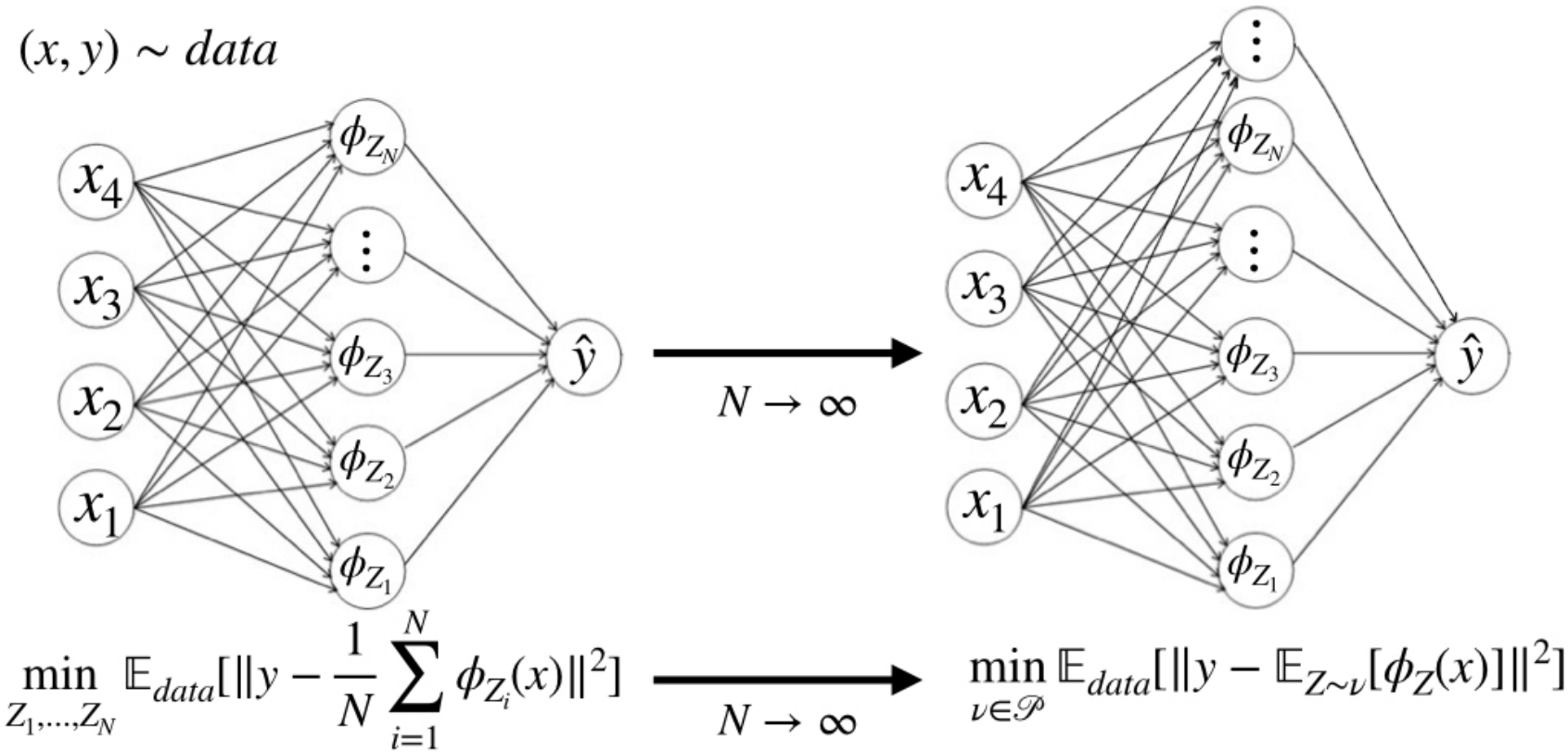


General problem

- Global convergence of Gradient descent[1] when $N \to \infty$ and $\phi_Z(x)$ of the form:

$$\phi_Z(x) = w g_\theta(x), \qquad Z = (w, \theta)$$



[1] [Rotskoff and Vanden-Eijnden, 2018, Chizat and Bach, 2018]

General problem

- Global convergence of Gradient descent[1] when $N \to \infty$ and $\phi_Z(x)$ of the form:

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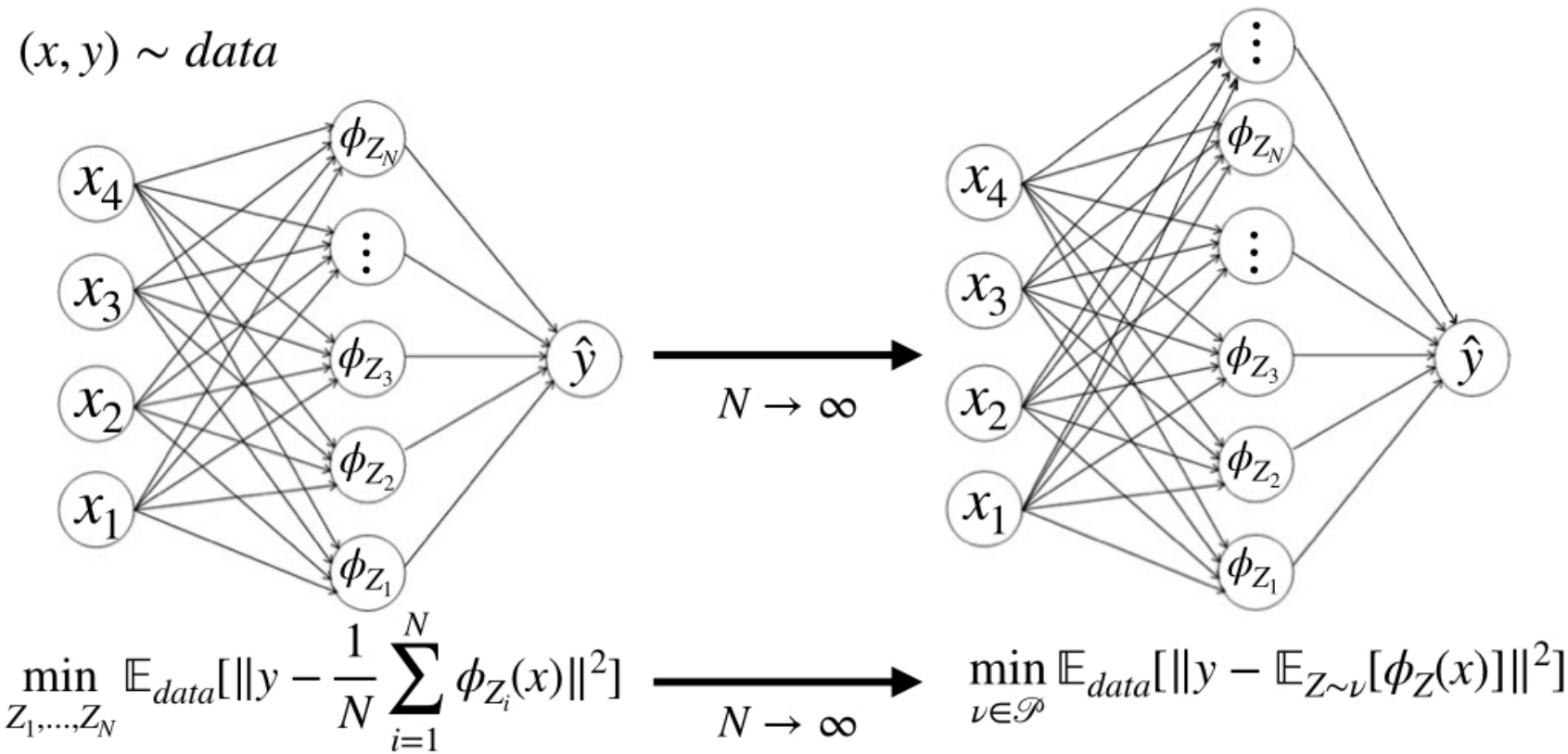
- Interested in more general form for $\phi_Z(x)$.



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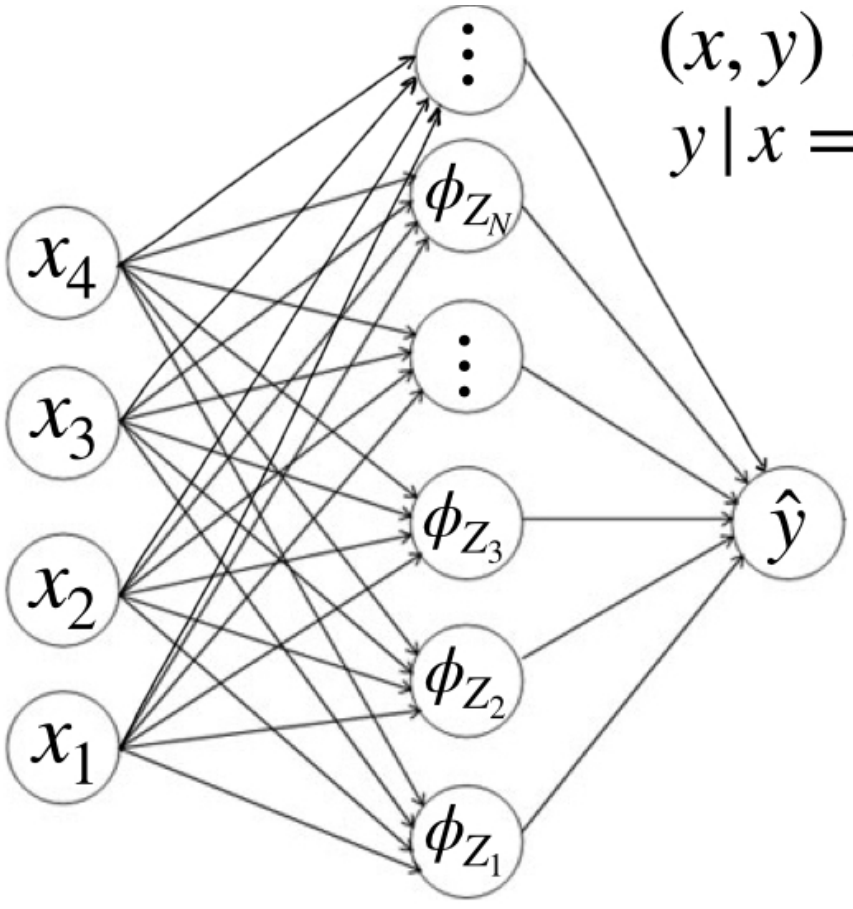
General problem

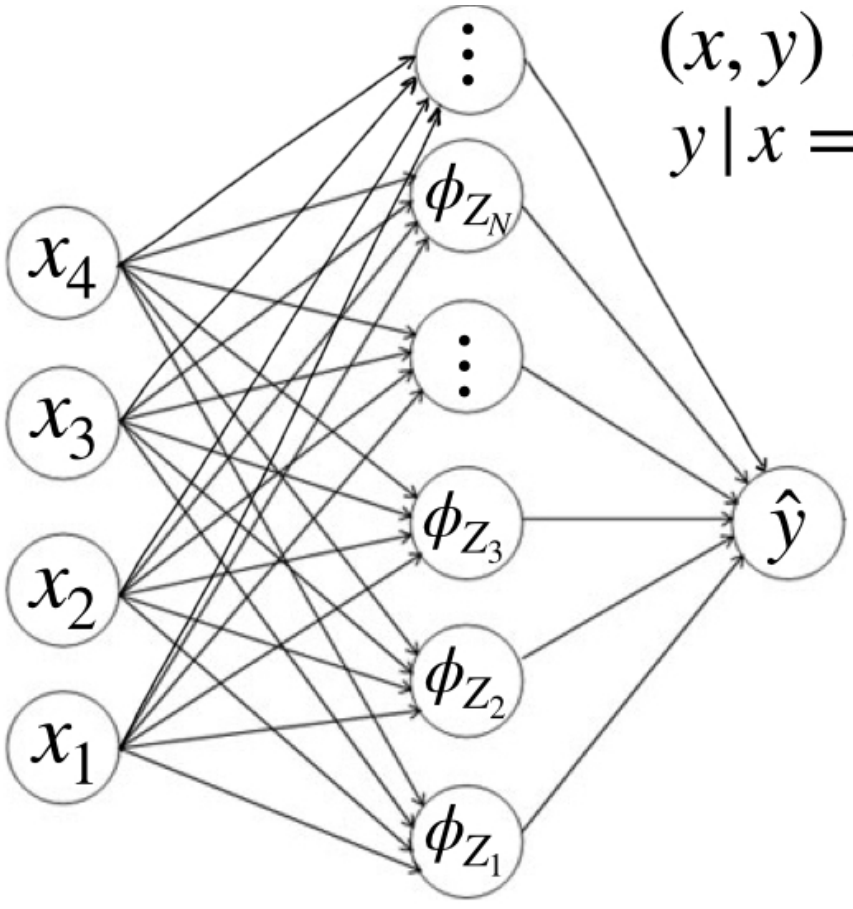


$$(x, y) \sim data$$

$$y \,|\, x = \mathbb{E}_{U \sim \nu^*}[\phi_U(x)]$$

$$\min_{\nu \in \mathcal{P}} \mathbb{E}_{data}[\|y - \mathbb{E}_{Z \sim \nu}[\phi_Z(x)]\|^2]$$

General problem



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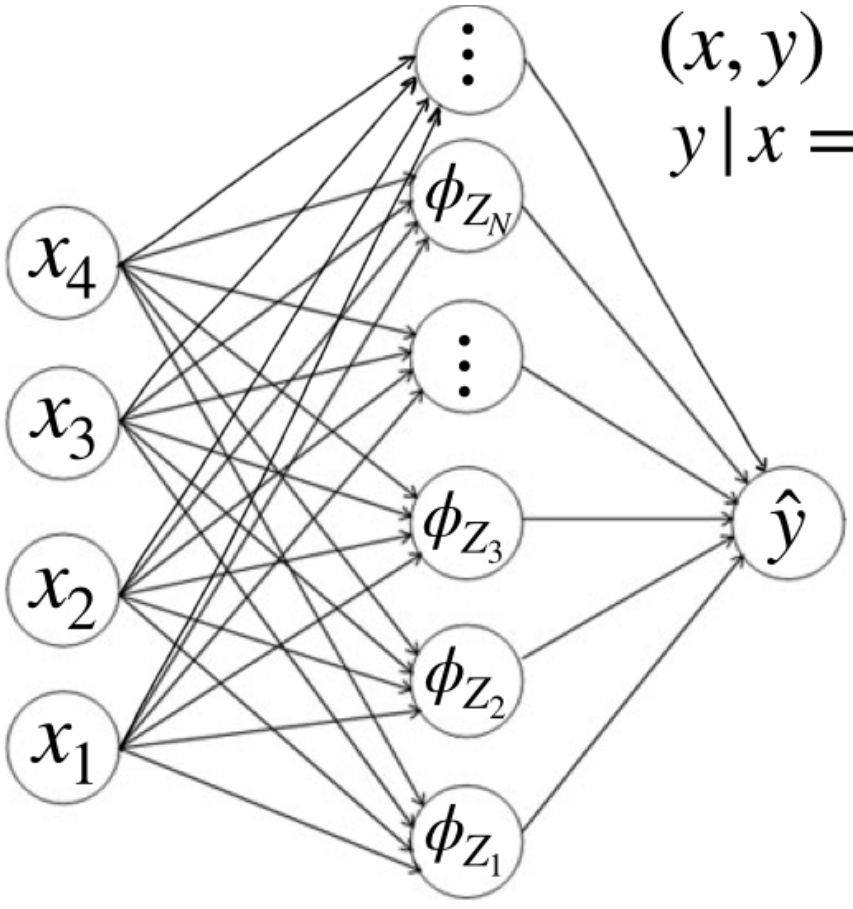
General problem



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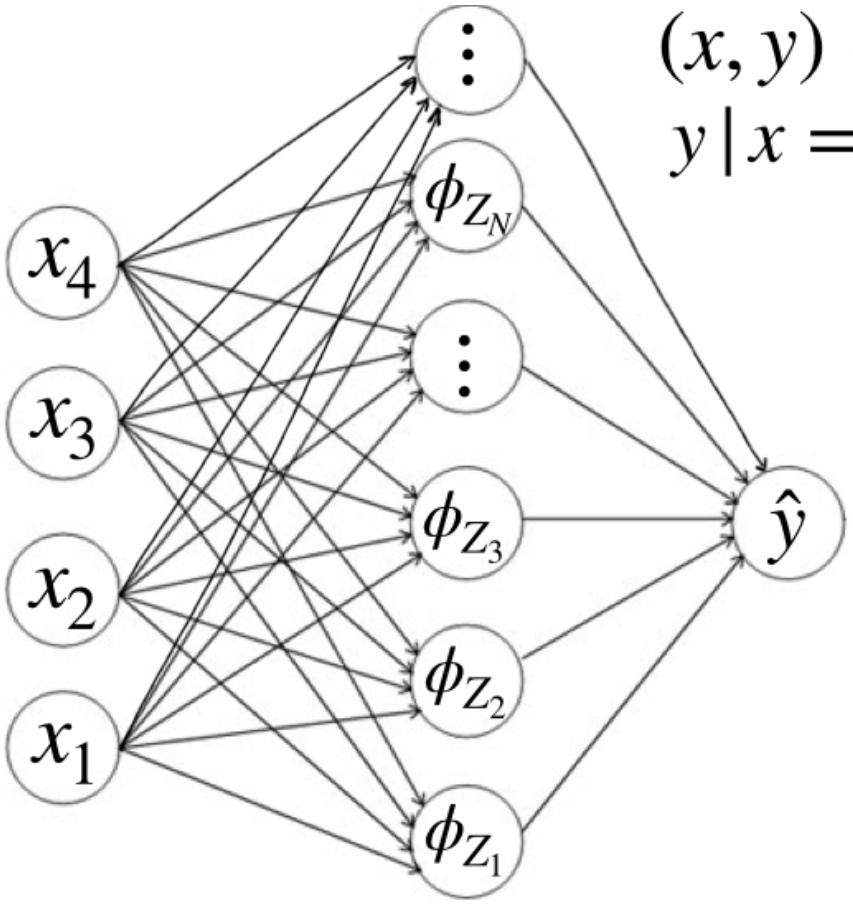


$$(x, y) \sim data$$

$$y \mid x = \mathbb{E}_{U \sim \nu^*}[\phi_U(x)]$$

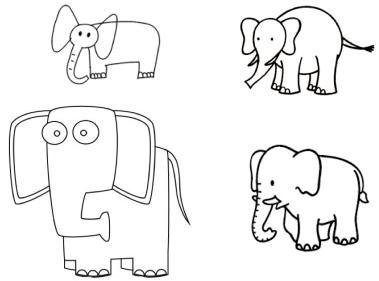
$$\min_{\nu \in \mathcal{P}} MMD^2(\nu^*, \nu)$$

$$k(Z, Z') = \mathbb{E}_{data}[\phi_Z(x)\phi_{Z'}(x)]$$

The Maximum Mean Discrepancy[2]

Consider samples from two distributions ν^* and ν_0.

$U^m \sim \nu^*$

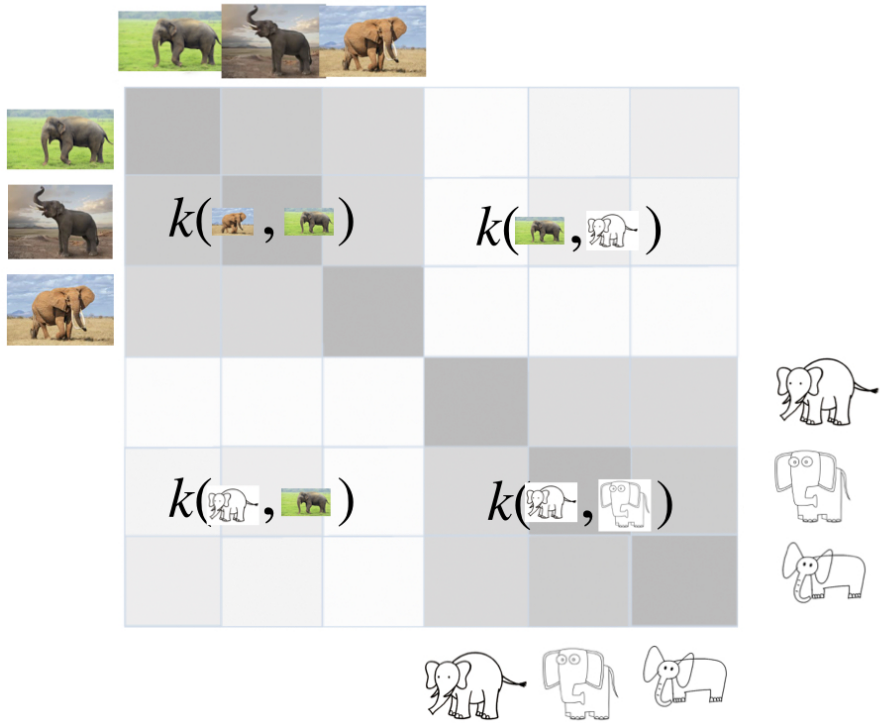


$Z^n \sim \nu_0$

[2] [Gretton et al., 2012]

The Maximum Mean Discrepancy[2]

Compute a similarity matrix using a kernel k



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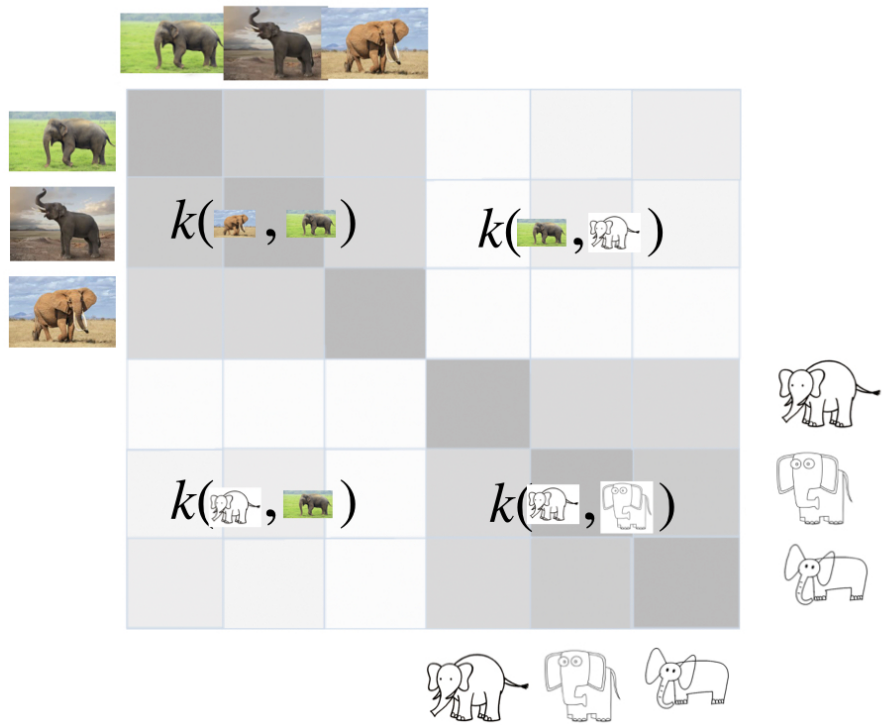
Compute a similarity matrix using a kernel *k*



$$\widehat{MMD}^2 = \frac{1}{n(n-1)} \sum_{n,n'} k(\,,\,) + \frac{1}{n(n-1)} \sum_{n,n'} k(\,,\,) - \frac{2}{n^2} \sum_{n,n'} k(\,,\,)$$

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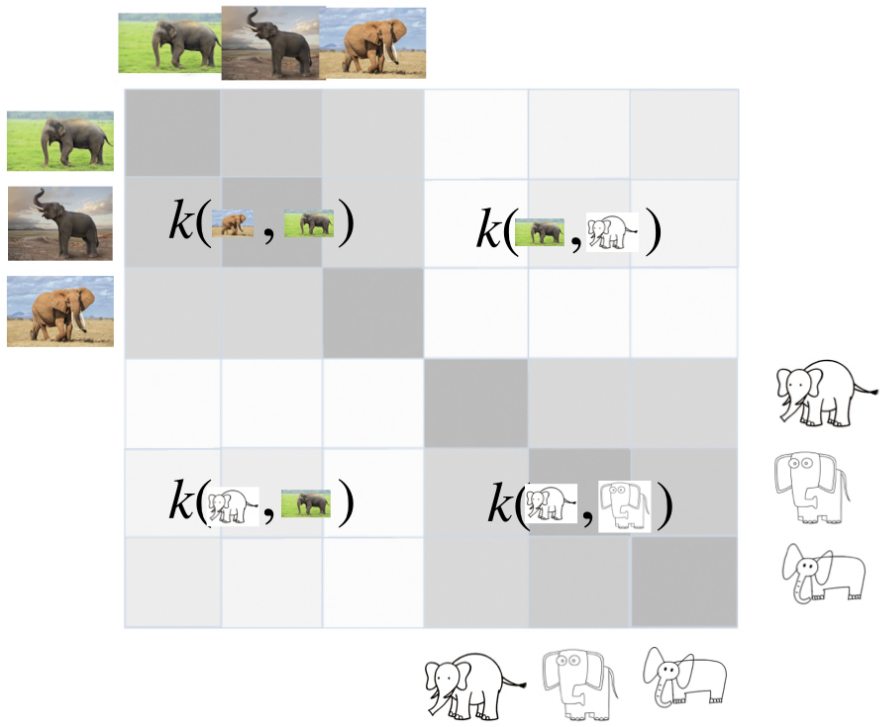

$$MMD^2(\nu^*, \nu_0) = \mathbb{E}_{\substack{U \sim \nu^* \\ U' \sim \nu^*}}[k(U, U')] + \mathbb{E}_{\substack{Z \sim \nu_0 \\ Z' \sim \nu_0}}[k(Z, Z')] - 2\mathbb{E}_{\substack{U \sim \nu^* \\ Z' \sim \nu_0}}[k(U, Z)]$$

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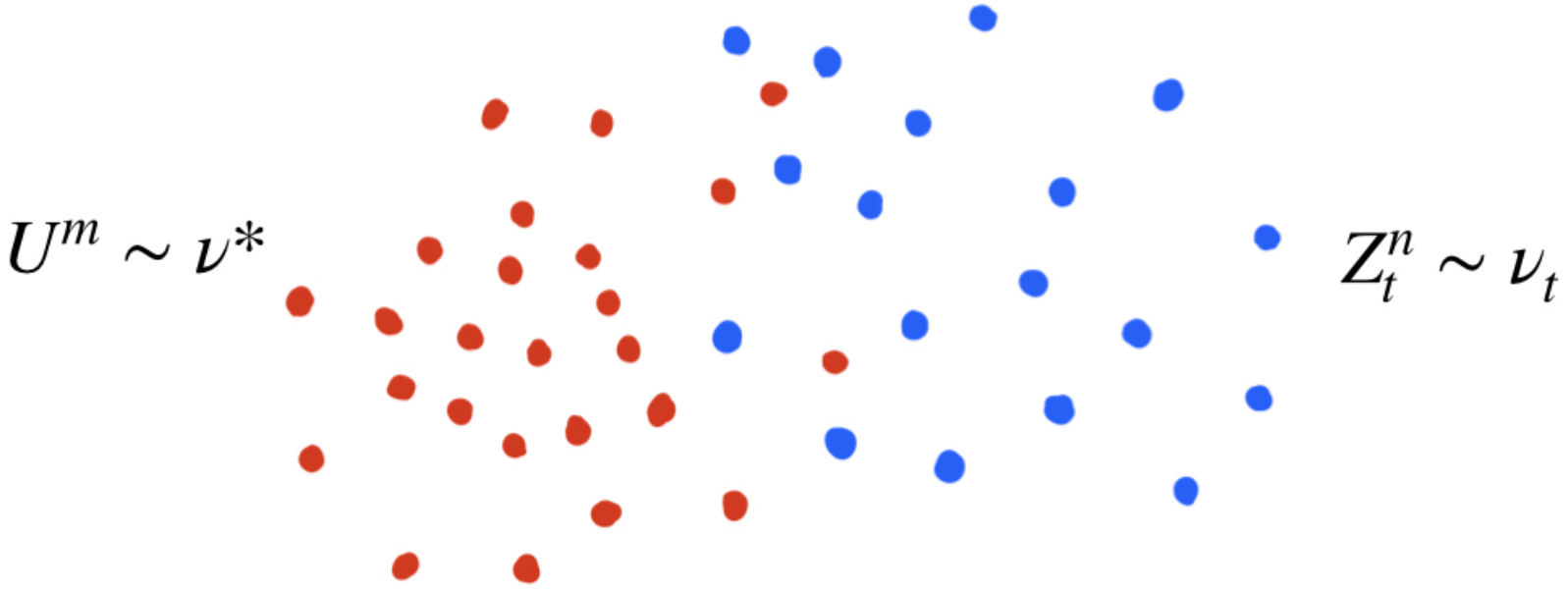
Gradient descent



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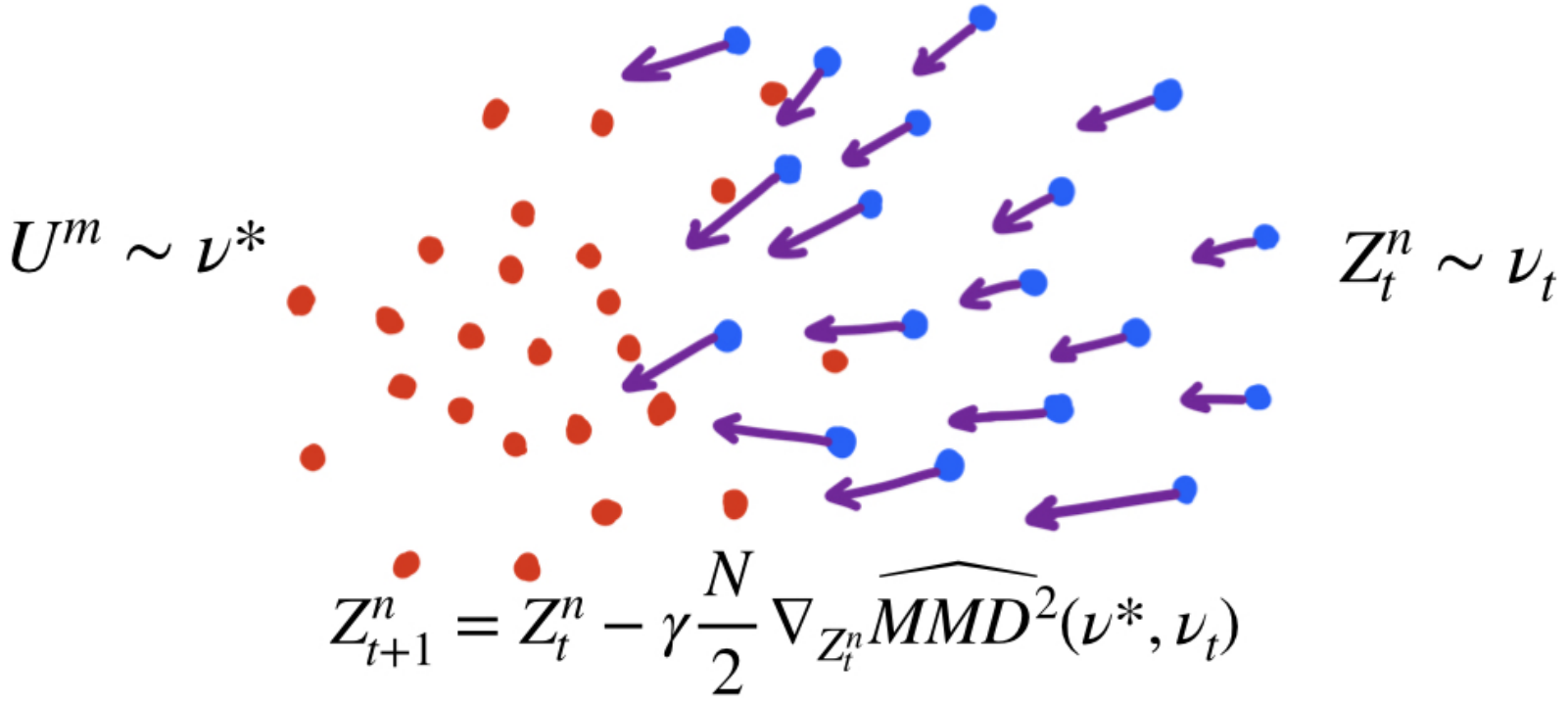

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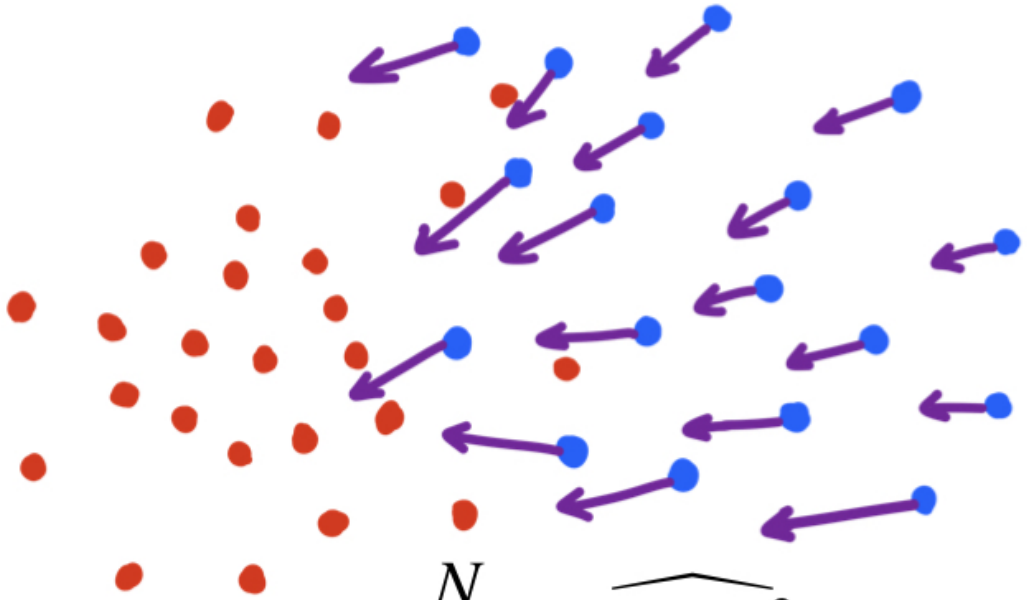

$$Z_{t+1}^n = Z_t^n - \gamma \frac{N}{2} \nabla_{Z_t^n} \widehat{MMD}^2(\nu^*, \nu_t)$$

$$\frac{N}{2} \nabla_{Z_t^n} \widehat{MMD}^2(\nu^*, \nu_t) = \frac{1}{N-1} \sum_{n' \neq n} \partial_1 k(Z_t^n, Z_t^{n'}) - \frac{1}{M} \sum_{m=1}^{M} \partial_1 k(Z_t^n, U^m)$$

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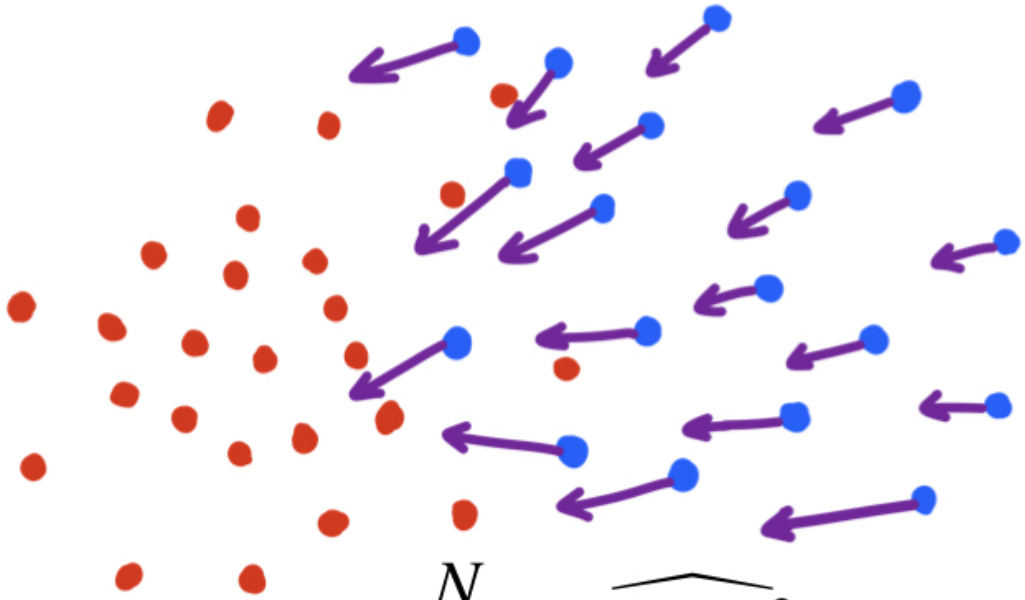

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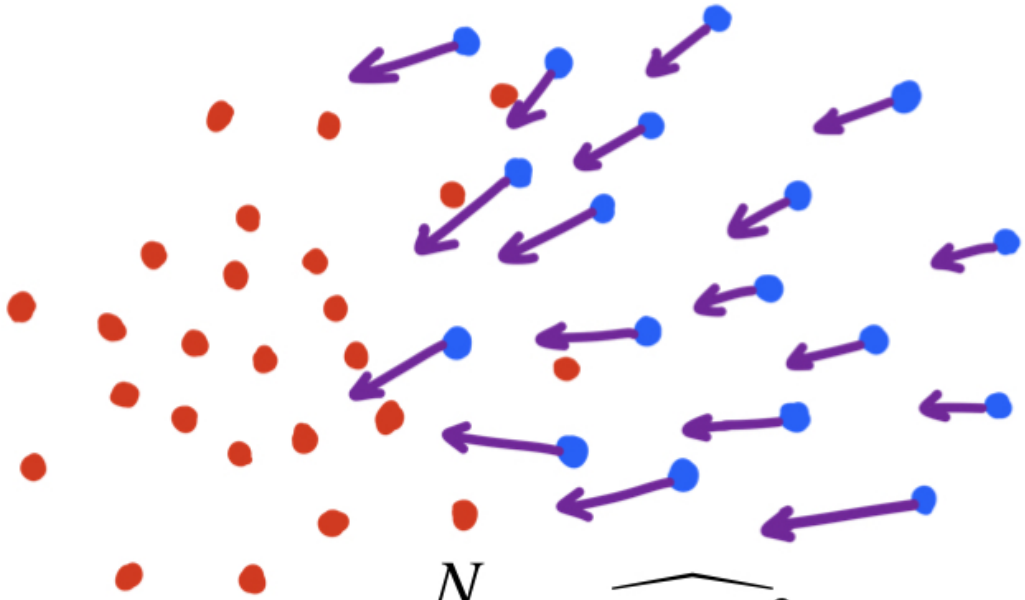
$$\downarrow N, M \to \infty$$

$$\nabla_{Z_t} \Big(\mathbb{E}_{Z' \sim \nu_t}[k(Z_t, Z')] - \mathbb{E}_{U \sim \nu^*}[k(Z_t, U)] \Big)$$

Gradient descent



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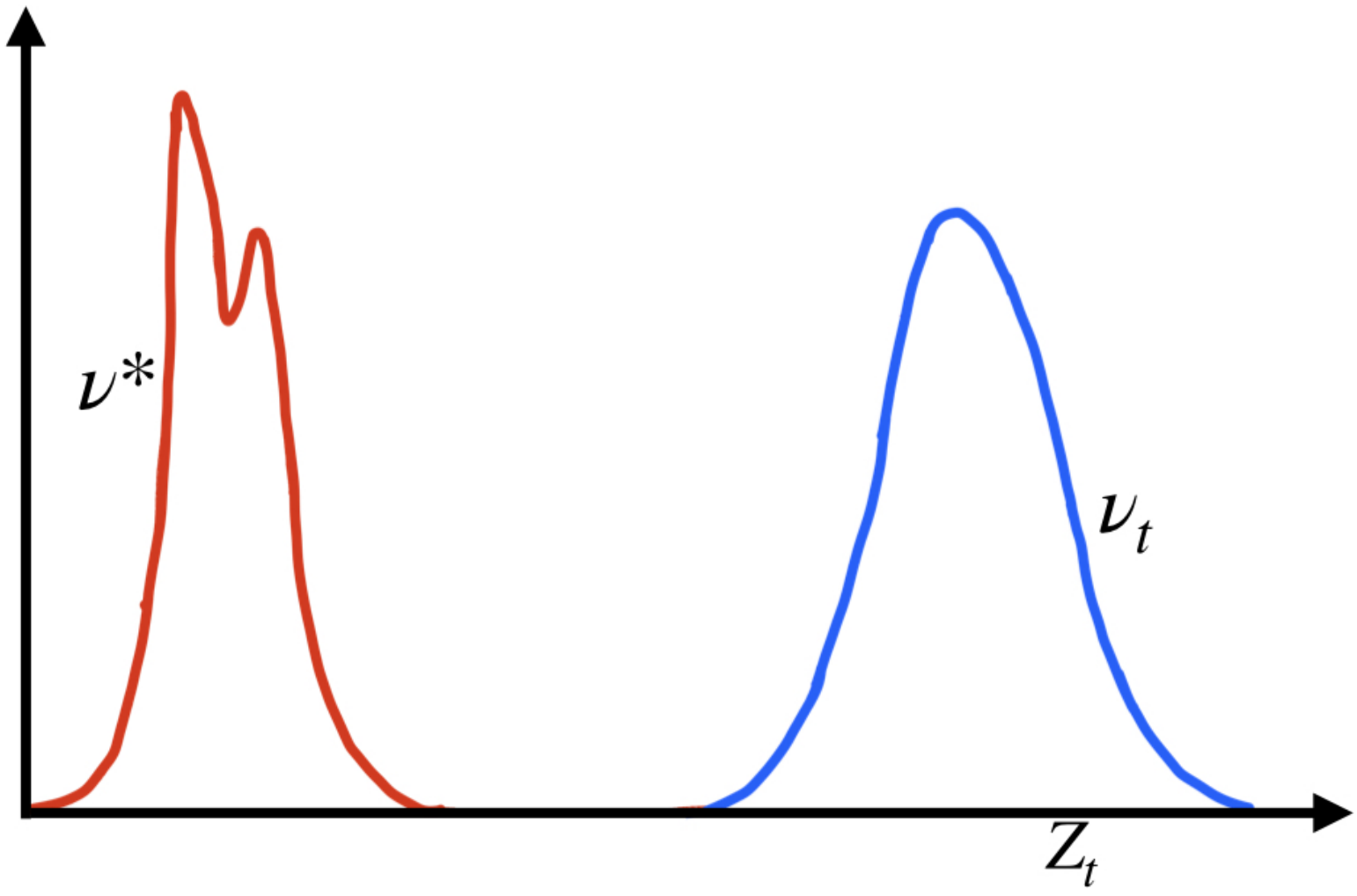
$$\nabla_{Z_t} \underbrace{\left(\mathbb{E}_{Z' \sim \nu_t}[k(Z_t, Z')] - \mathbb{E}_{U \sim \nu^*}[k(Z_t, U)] \right)}_{f_{\nu^*, \nu_t}(Z_t)}$$

Wasserstein gradient descent



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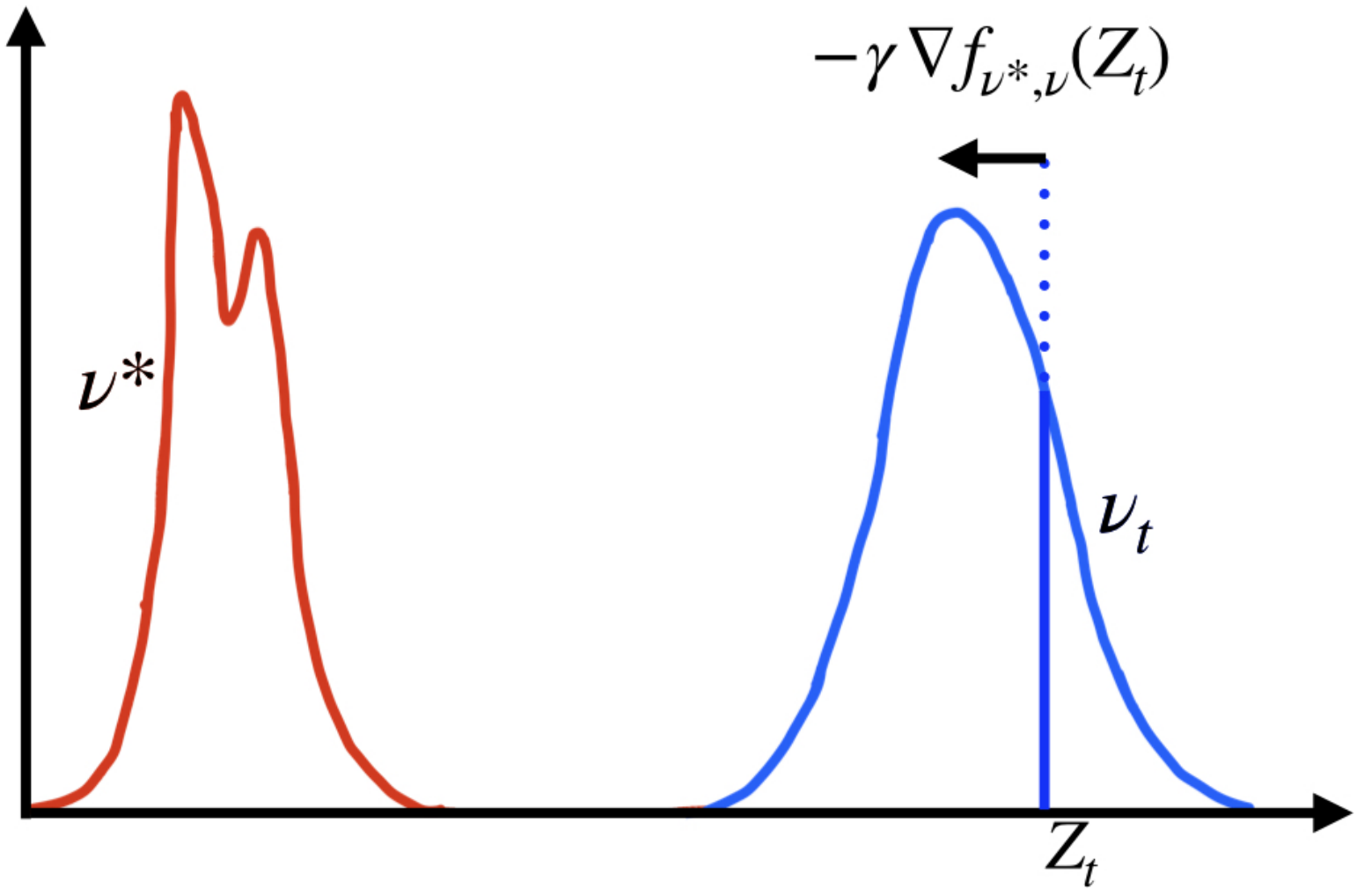
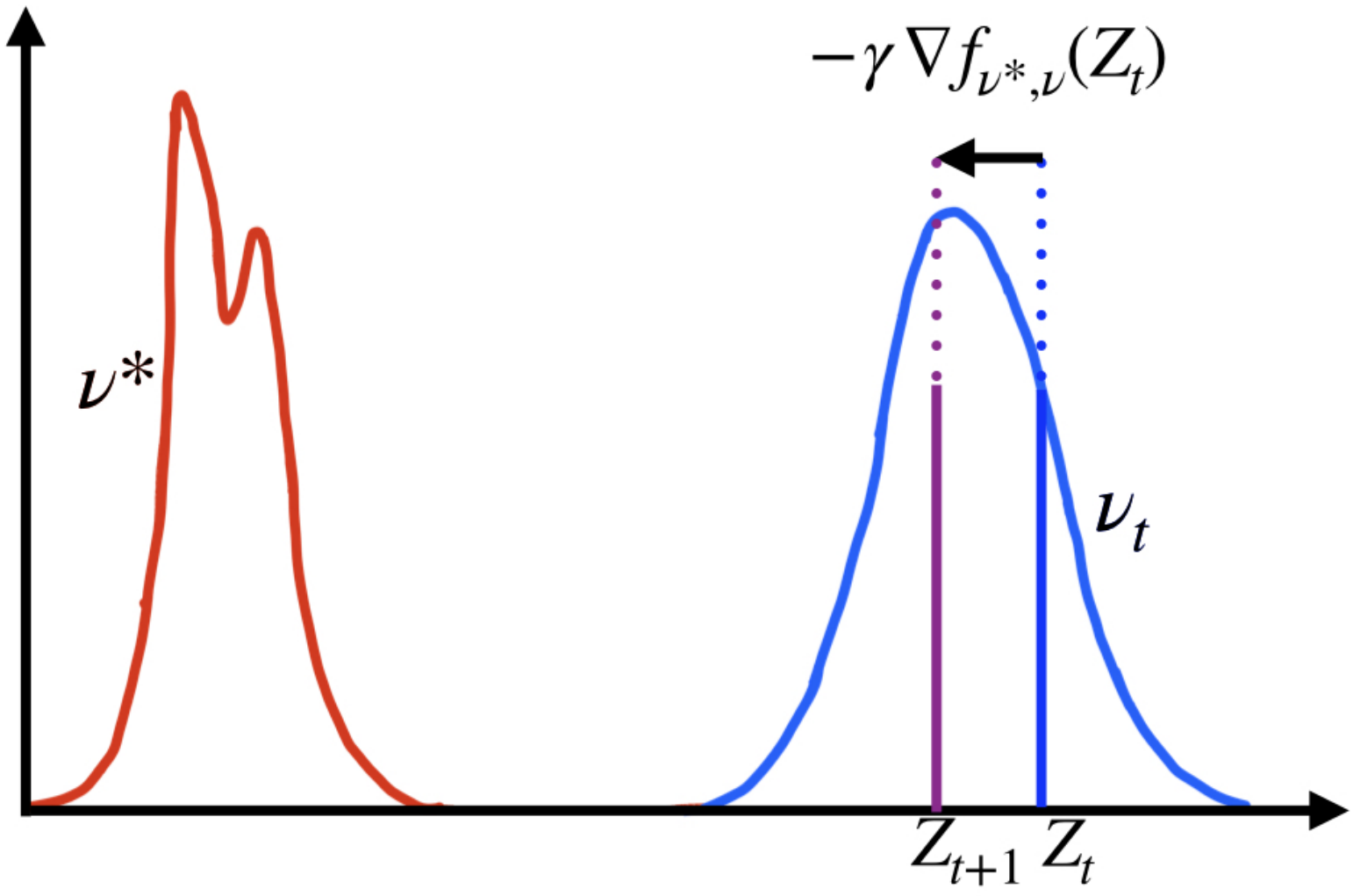


$$f_{\nu^*,\nu_t}(Z_t) = \mathbb{E}_{Z' \sim \nu_t}[k(Z_t, Z')] - \mathbb{E}_{U \sim \nu^*}[k(Z_t, U)]$$

Wasserstein gradient descent



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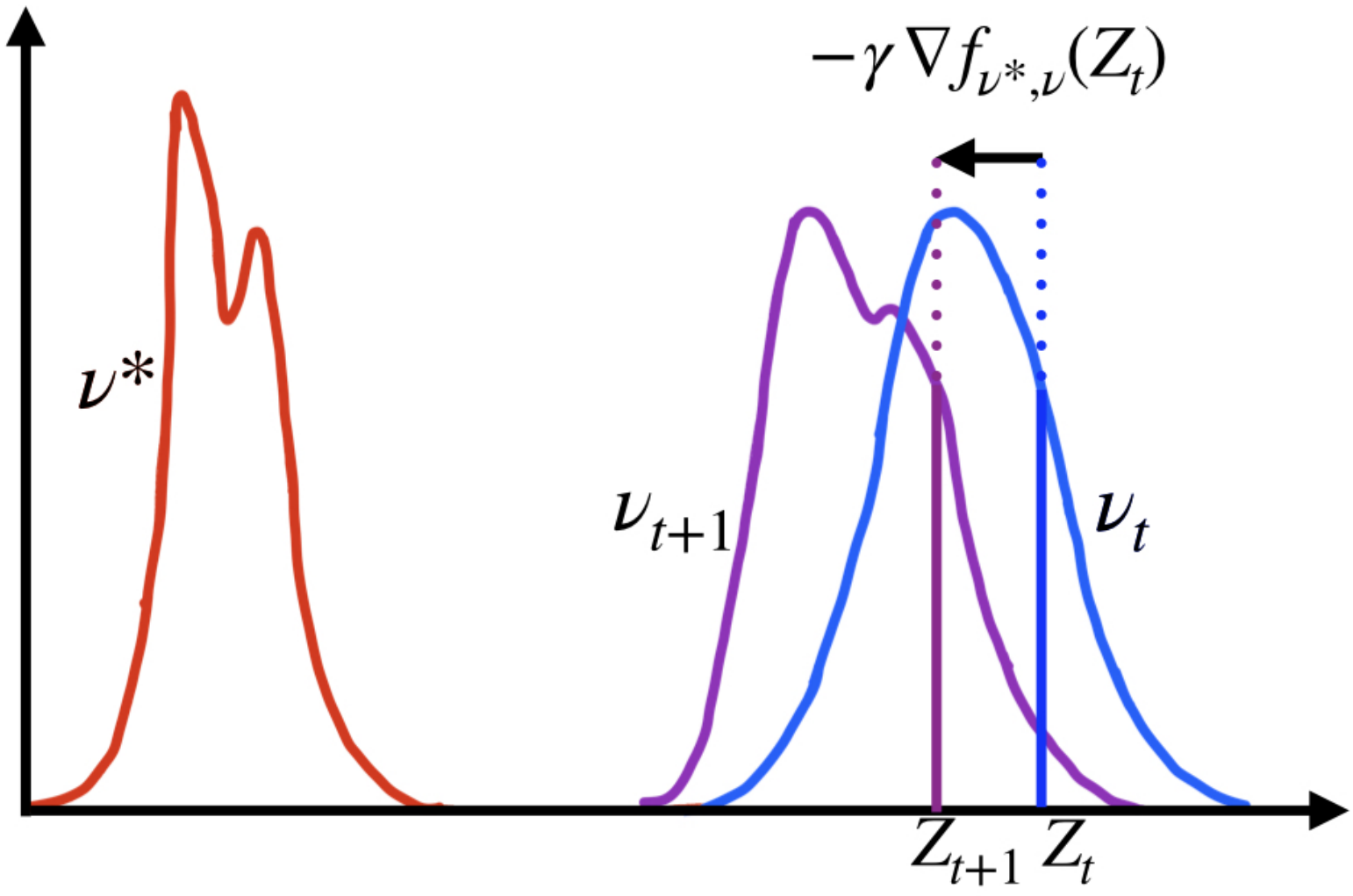

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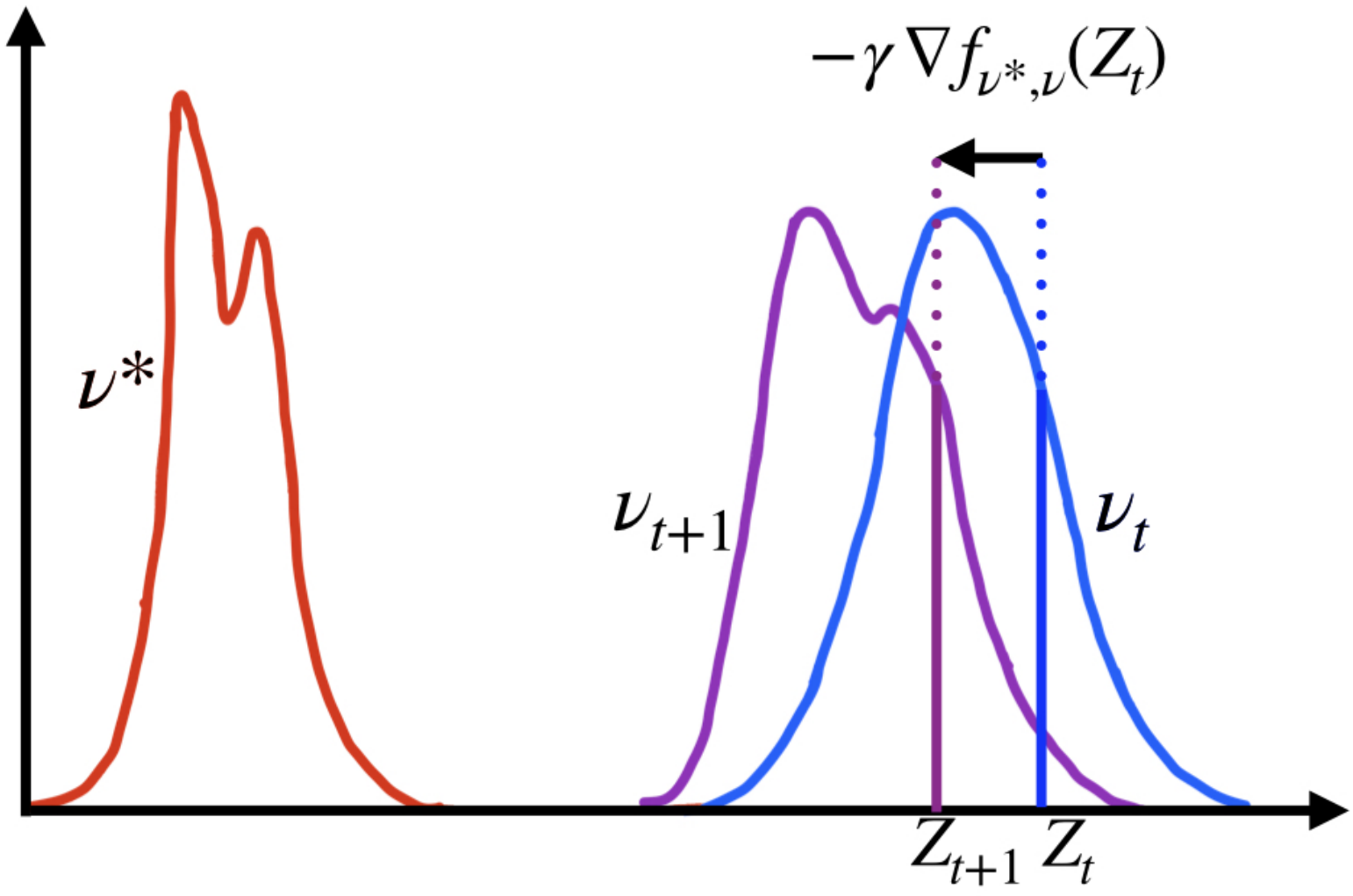
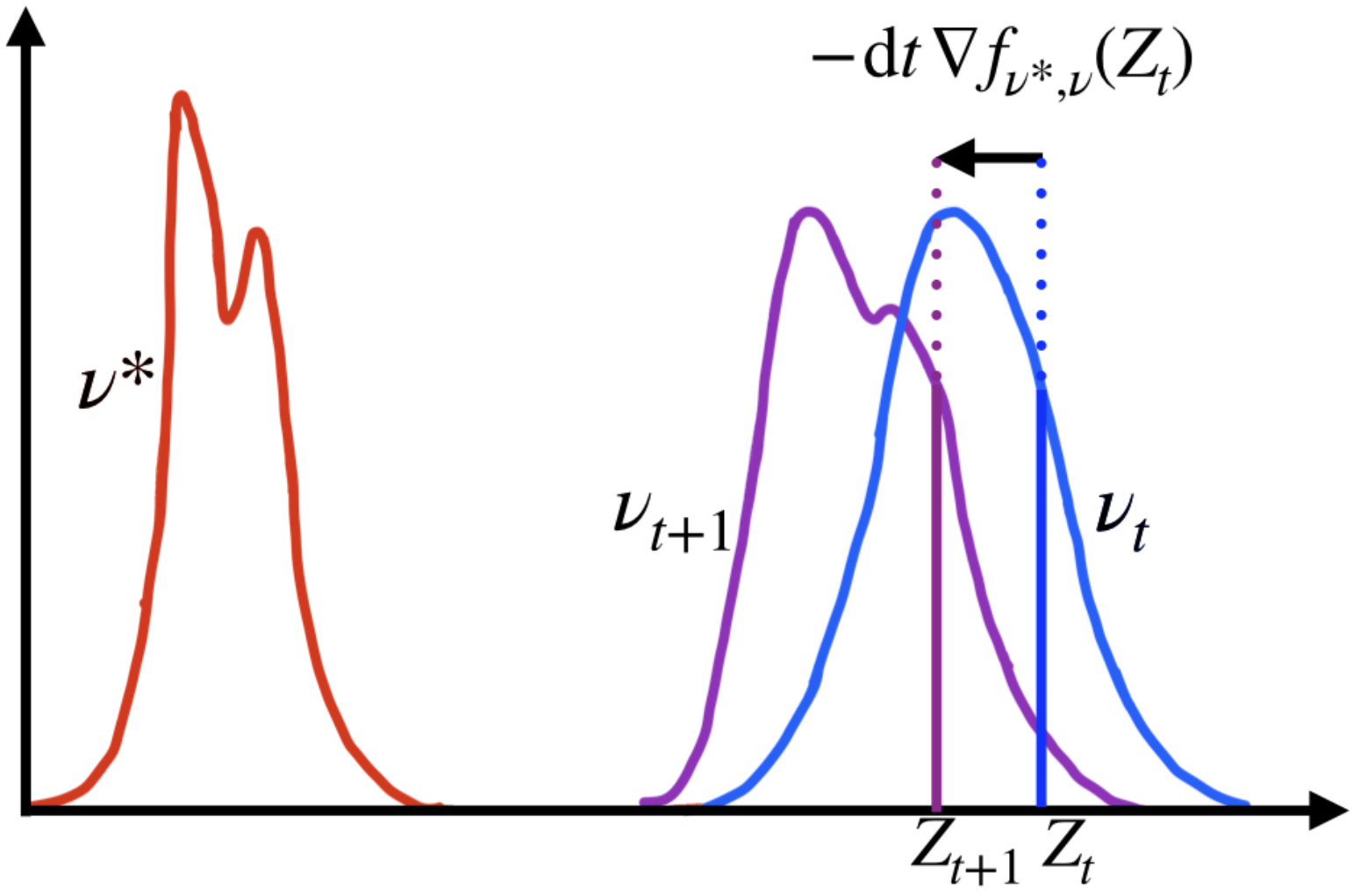


$$Z_{t+1} = Z_t - \gamma \nabla_{Z_t} f_{\nu^*,\nu_t}(Z_t), \qquad Z_t \sim \nu_t$$

Wasserstein gradient descent



$$\mathrm{d}Z_t = -\,\mathrm{d}t\,\nabla_{Z_t} f_{\nu^*,\nu_t}(Z_t), \qquad Z_t \sim \nu_t$$

Wasserstein gradient flow

Continuity Equation

- Continuous time equation: Mc-Kean Vlasov dynamics

$$\frac{\mathrm{d}Z_t}{\mathrm{d}t} = -\nabla_{Z_t} f_{\nu^*,\nu_t}(Z_t), \qquad Z_t \sim \nu_t$$

[3] [Otto, 2001, Villani, 2004, Ambrosio et al., 2004]

Continuity Equation

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- Equivalent to a PDE in ν_t:

$$\partial_t \nu_t = \mathit{div}(\nu_t \nabla f_{\nu^*,\nu_t})$$

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- Interpretation as a gradient flow in probability space [3]:

$$\partial_t \nu_t = -\nabla_{\nu_t} \mathcal{L}(\nu_t) \qquad \mathcal{L}(\nu) := \frac{1}{2} \mathit{MMD}^2(\nu^*, \nu)$$

[3] [Otto, 2001, Villani, 2004, Ambrosio et al., 2004]

A criterion for convergence

- Define the Negative Sobolev distance:

$$S(\nu^*|\nu_t) = \sup_{g, \mathbb{E}_{Z\sim\nu_t}[\|\nabla g(Z)\|^2]\leq 1} |\mathbb{E}_{Z\sim\nu_t}[g(Z)] - \mathbb{E}_{U\sim\nu^*}[g(U)]|$$

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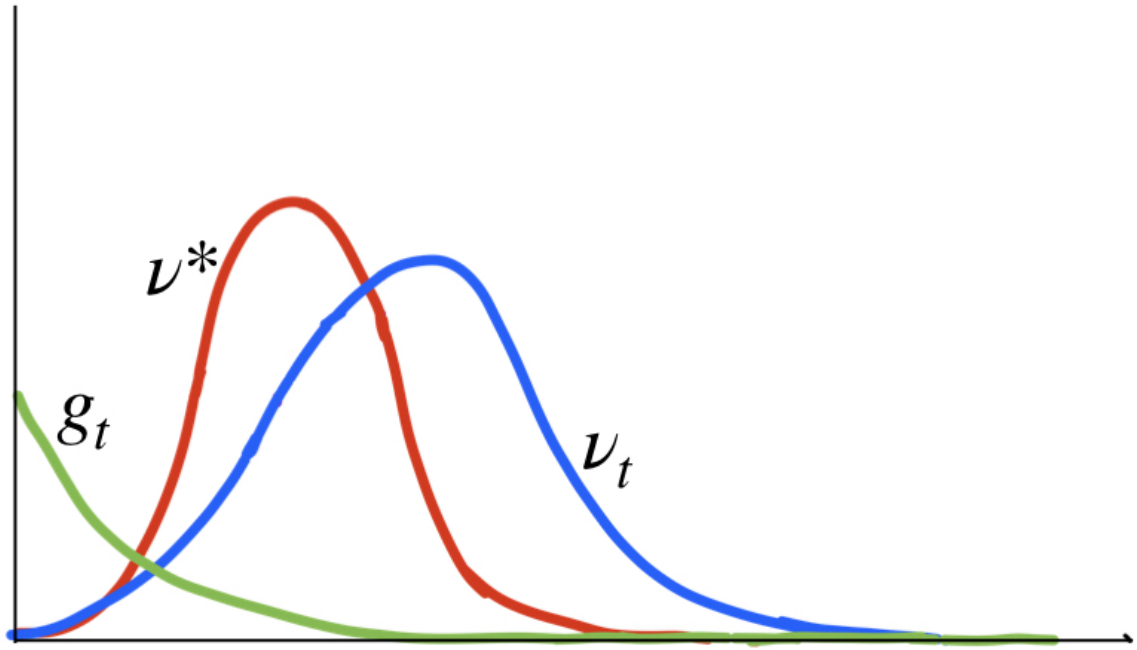

$$\int \|\nabla g_t(x)\|^2 \, d\nu_t(x) \leq 1$$

$$S(\nu^* \,|\, \nu_t) = |\, \mathbb{E}_{Z\sim\nu_t}[g_t(Z)] - \mathbb{E}_{U\sim\nu^*}[g_t(U)] \,|$$

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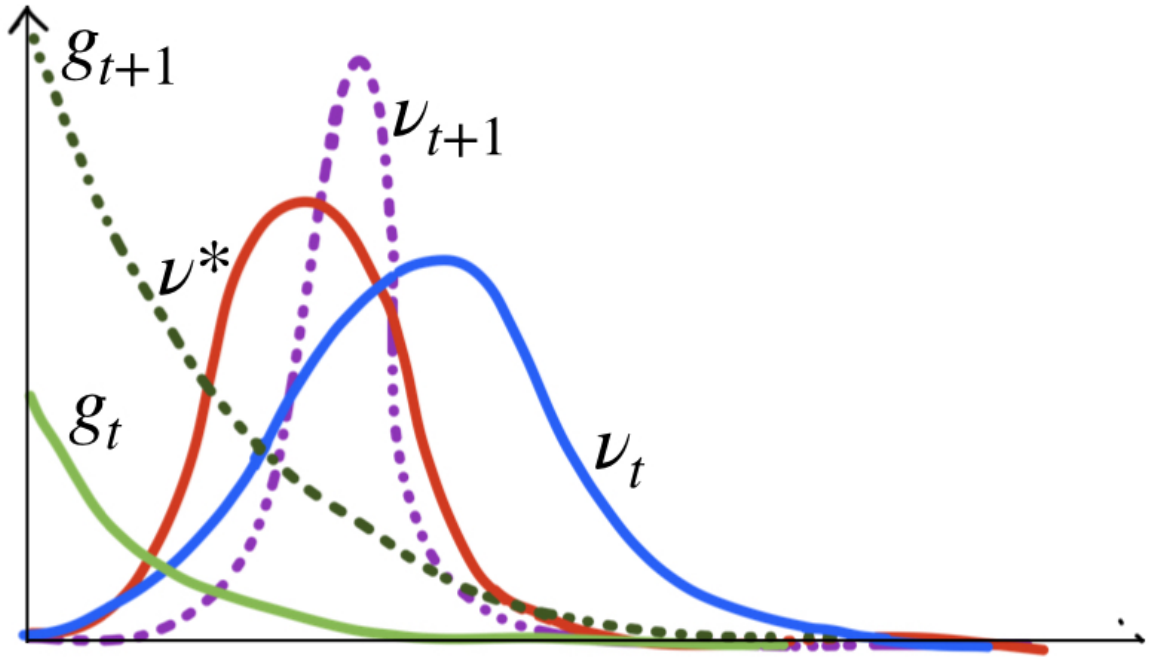

$$S(\nu^* \,|\, \nu_{t+1}) - S(\nu^* \,|\, \nu_t) > 0$$

A criterion for convergence

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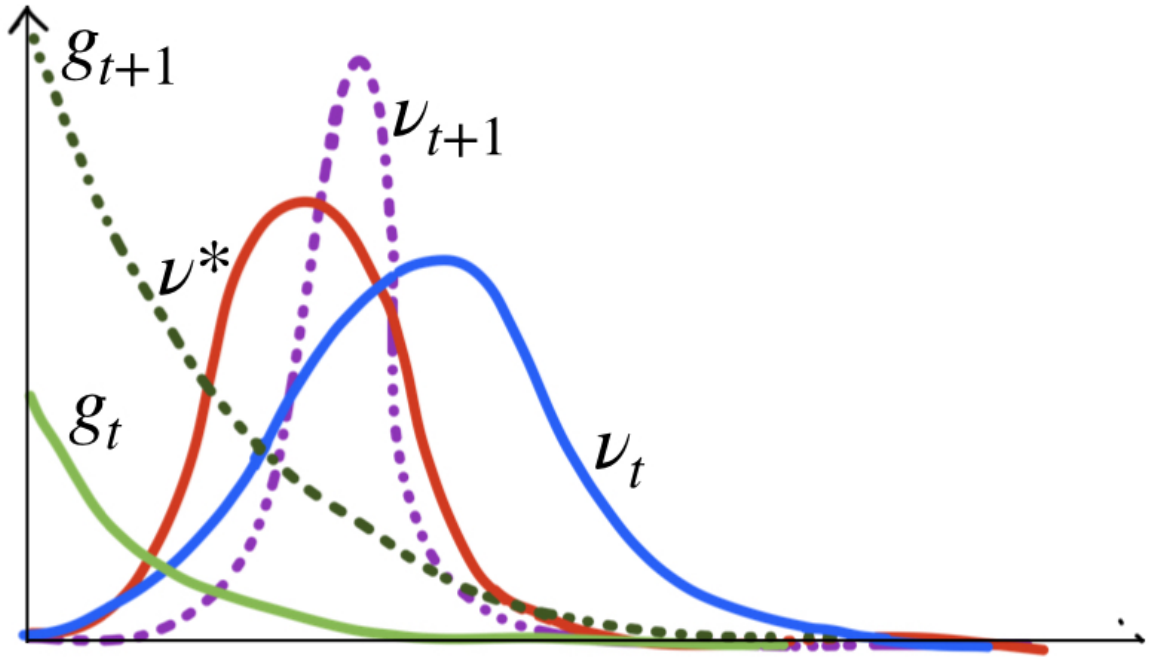

$$S(\nu^* \,|\, \nu_{t+1}) - S(\nu^* \,|\, \nu_t) > C$$

A criterion for convergence

- Assume that $S(\nu^*|\nu_t) \leq C$ for all t, then for γ small enough

$$MMD^2(\nu^*, \nu_t) \leq \frac{1}{MMD^2(\nu^*, \nu_0) + 8\gamma C^{-1} t}$$

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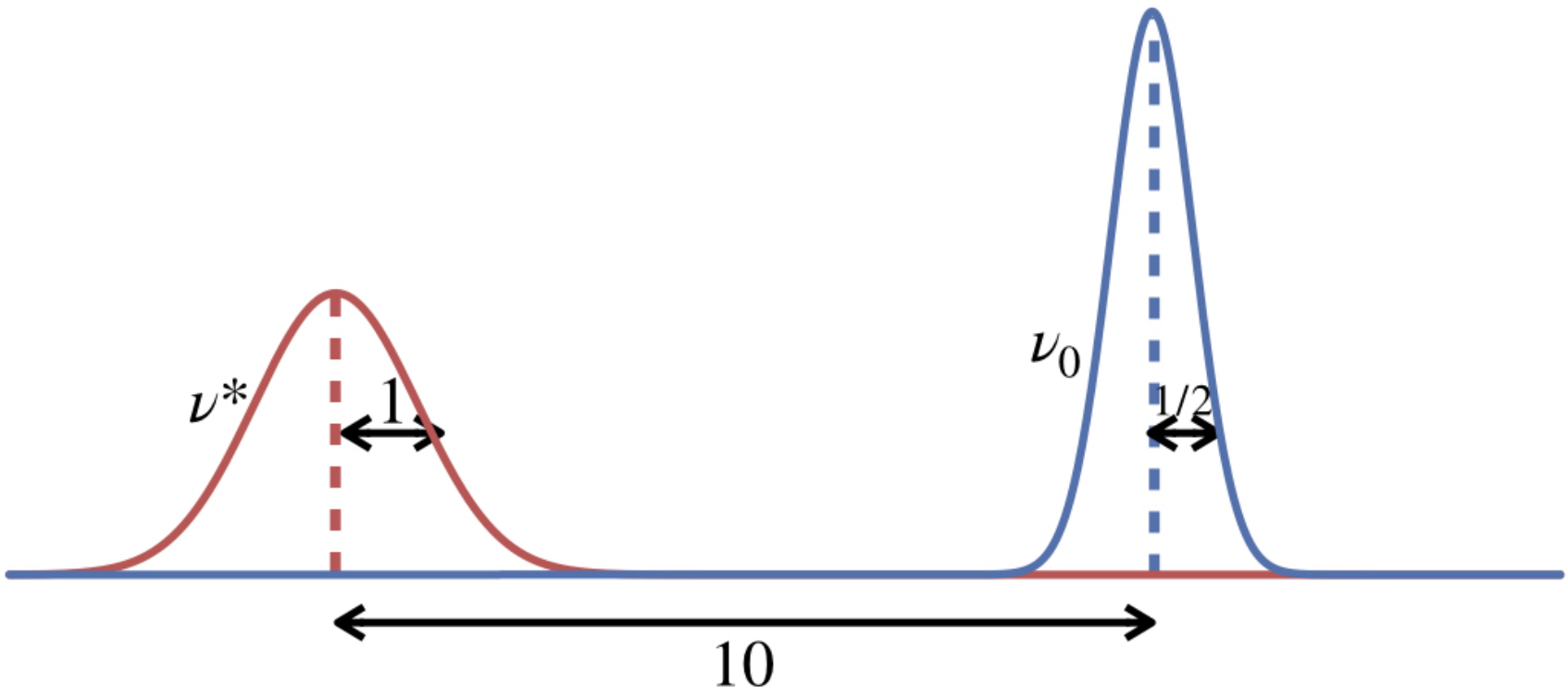
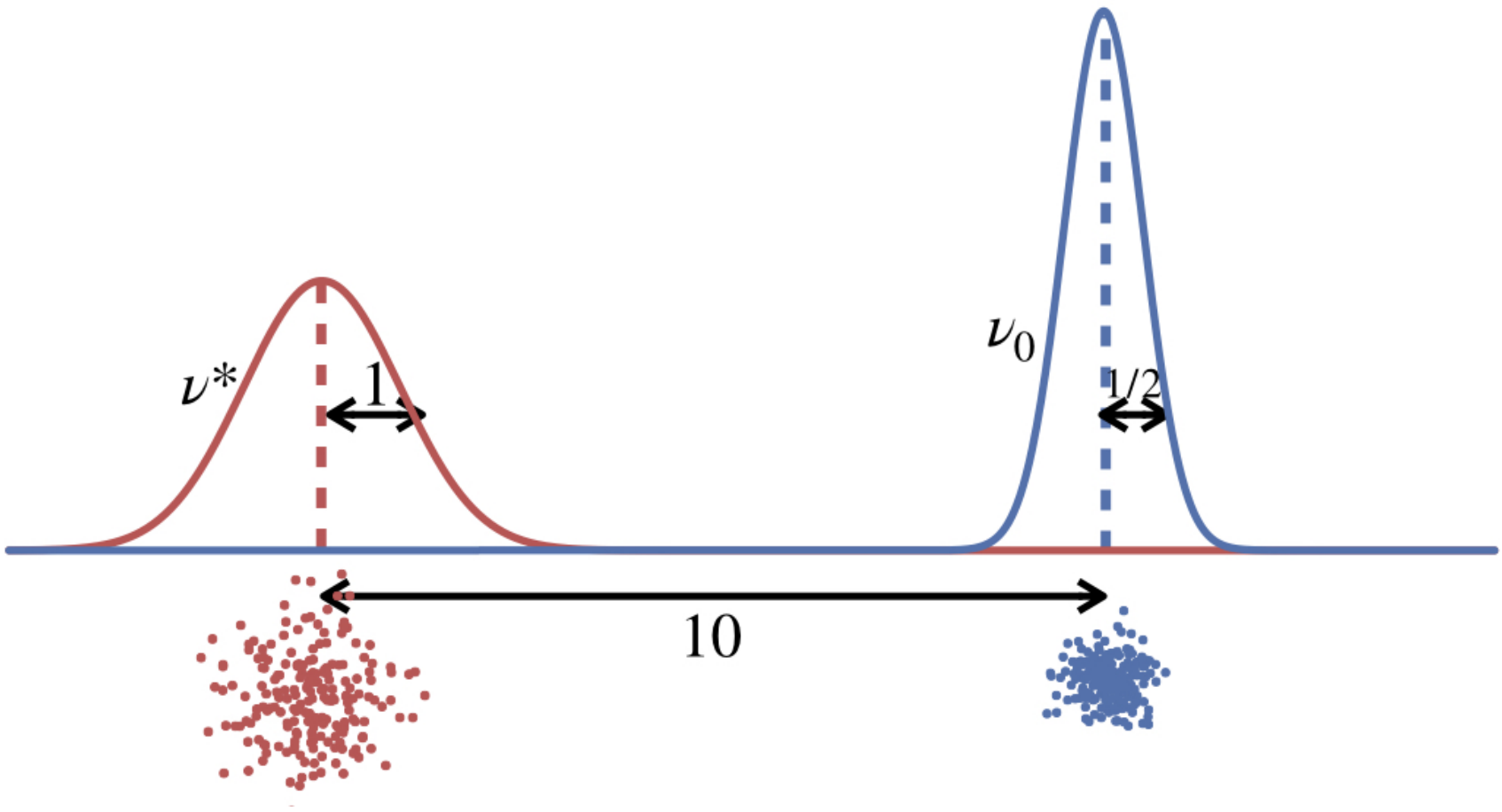
$$MMD^2(\nu^*, \nu_t) \leq \frac{1}{MMD^2(\nu^*, \nu_0) + 8\gamma C^{-1} t}$$

- Depends on the whole sequence ν_t: Hard to verify in general
- Can be checked for simple examples.

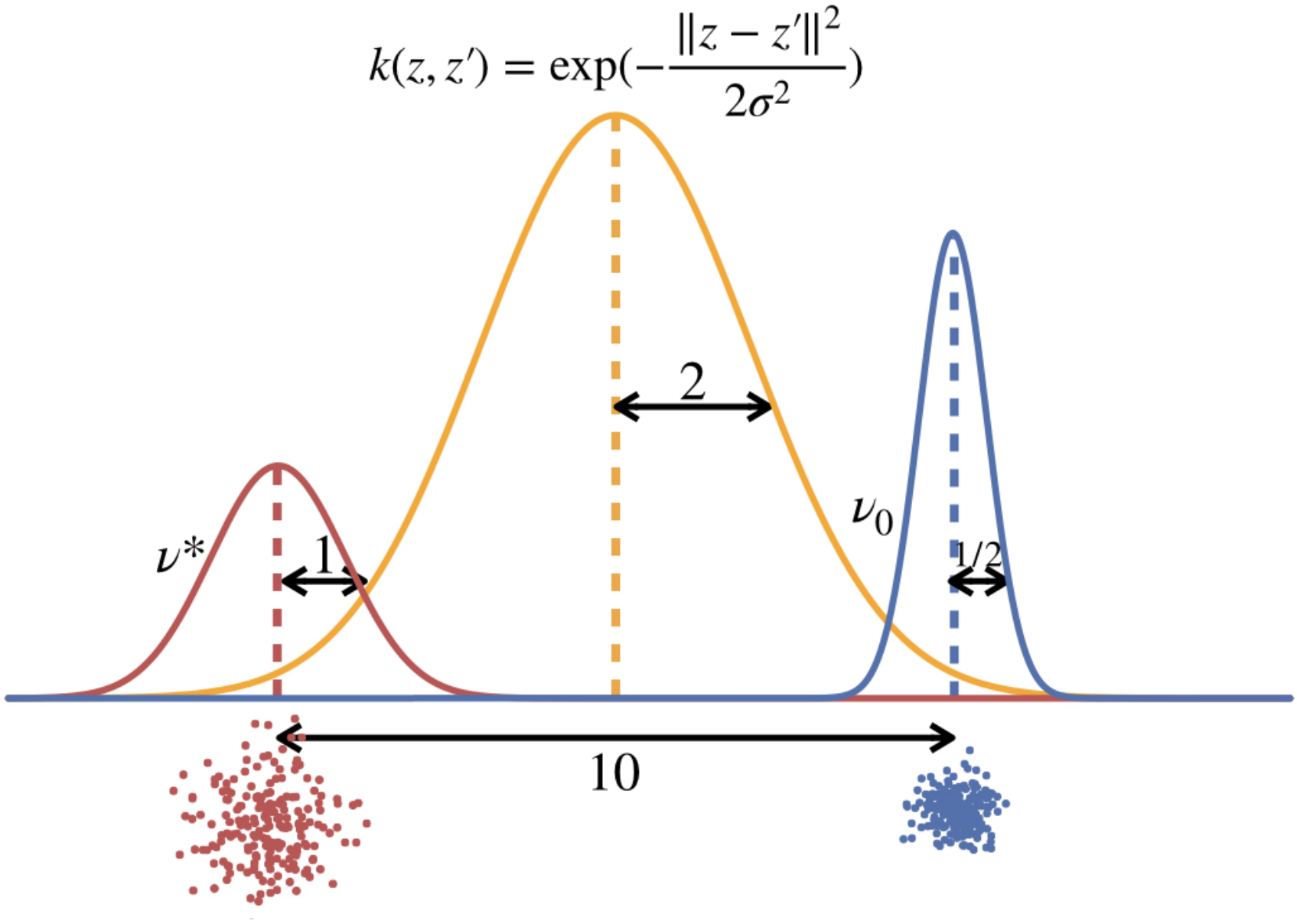
Convergence: Failure case



Convergence: Failure case



Convergence: Failure case



Convergence: Failure case

Noise Injection

- Idea: Evaluate $\nabla f_{\nu^*,\nu_t}$ outside of the support of ν_t to get a better signal!

[4] [Chaudhari et al., 2017, Hazan et al., 2015]

[5] [Mei et al., 2018]

Noise Injection

- Idea: Evaluate $\nabla f_{\nu^*,\nu_t}$ outside of the support of ν_t to get a better signal!
- Sample $u_t \sim \mathcal{N}(0,1)$ and β_t is the noise level:

$$Z_{t+1} = Z_t - \gamma \nabla f_t(Z_t + \beta_t u_t); \qquad Z_t \sim \nu_t$$

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- Similar to *continuation methods* [4], but extended to interacting particles.
- Different from entropic regularization[5]

$$Z_{t+1} = Z_t - \gamma \nabla f_{\nu^*,\nu_t}(Z_t) + \beta_t u_t$$

[4] [Chaudhari et al., 2017, Hazan et al., 2015]

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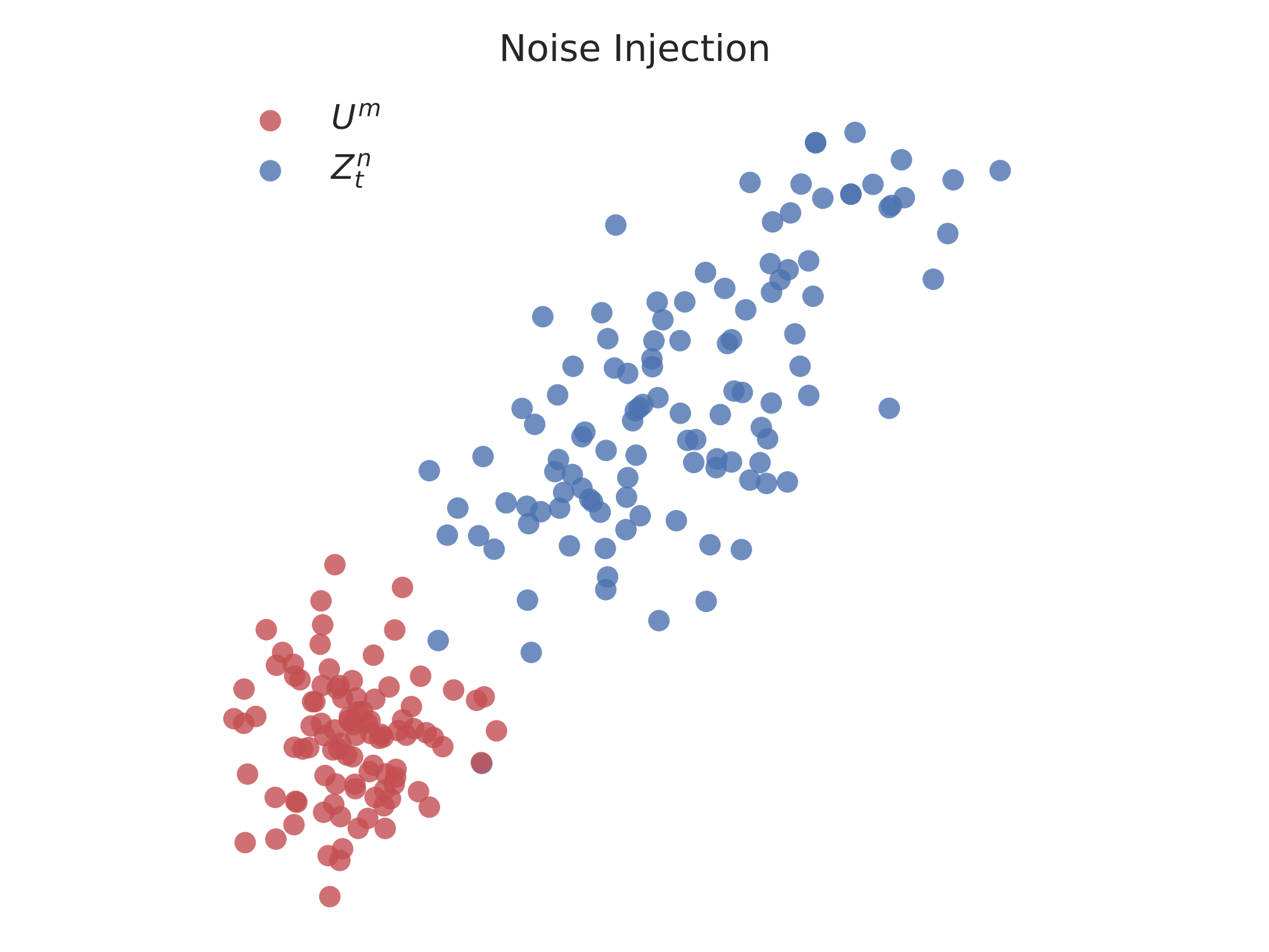
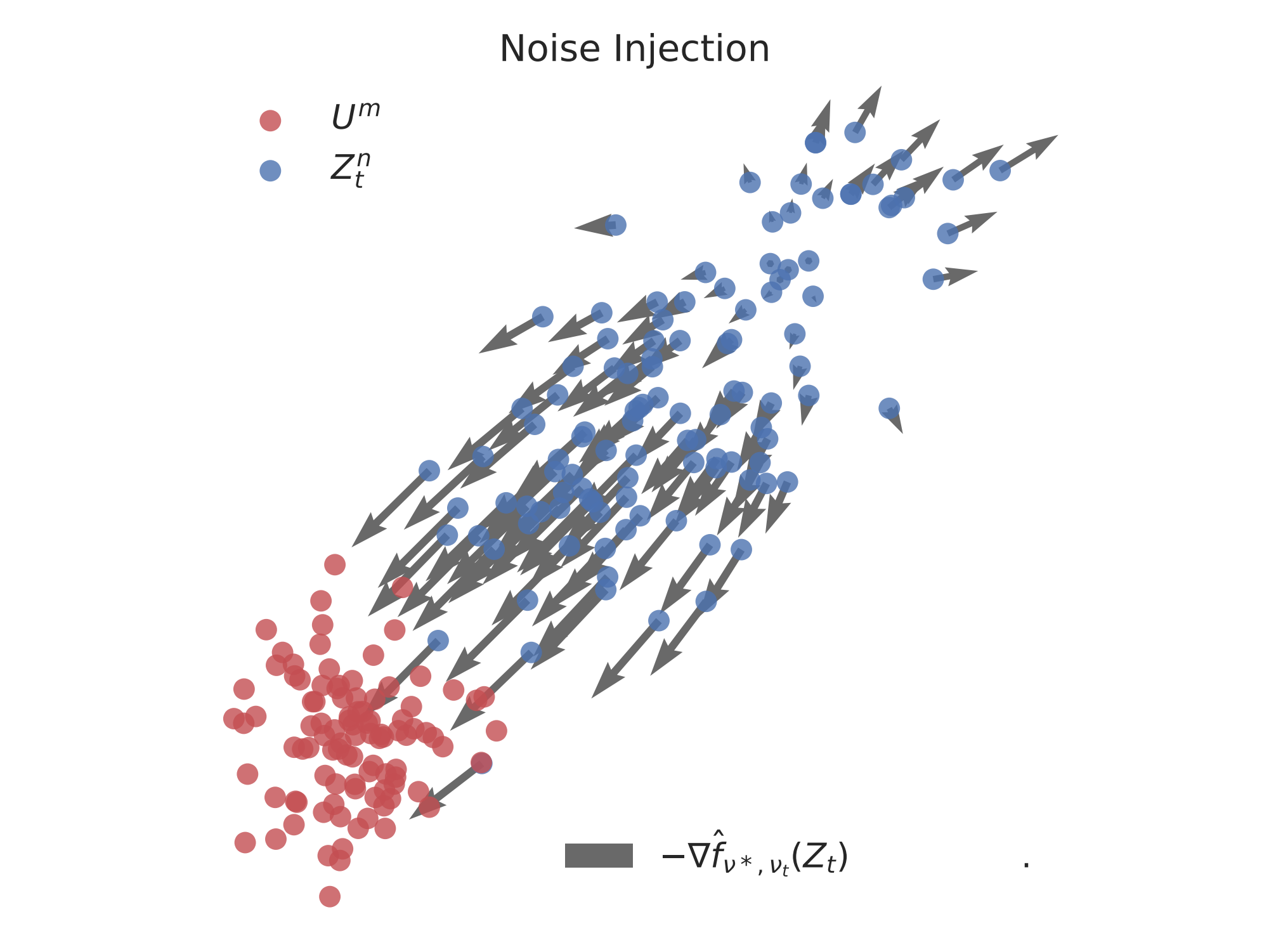
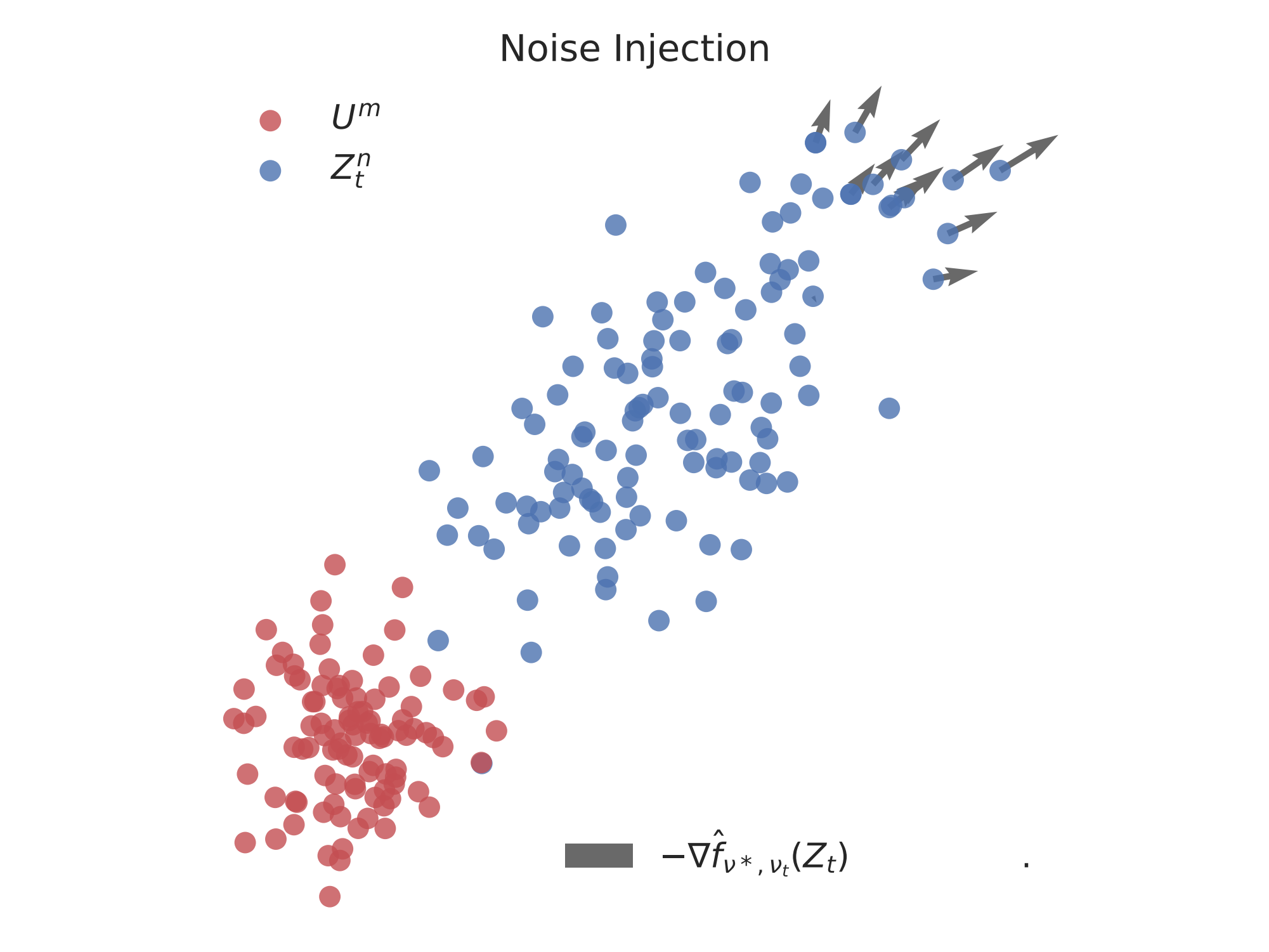

Noise Injection
U^m
Z_t^n


Noise Injection
U^m
Z_t^n
$-\nabla \hat{f}_{\nu^*, \nu_t}(Z_t)$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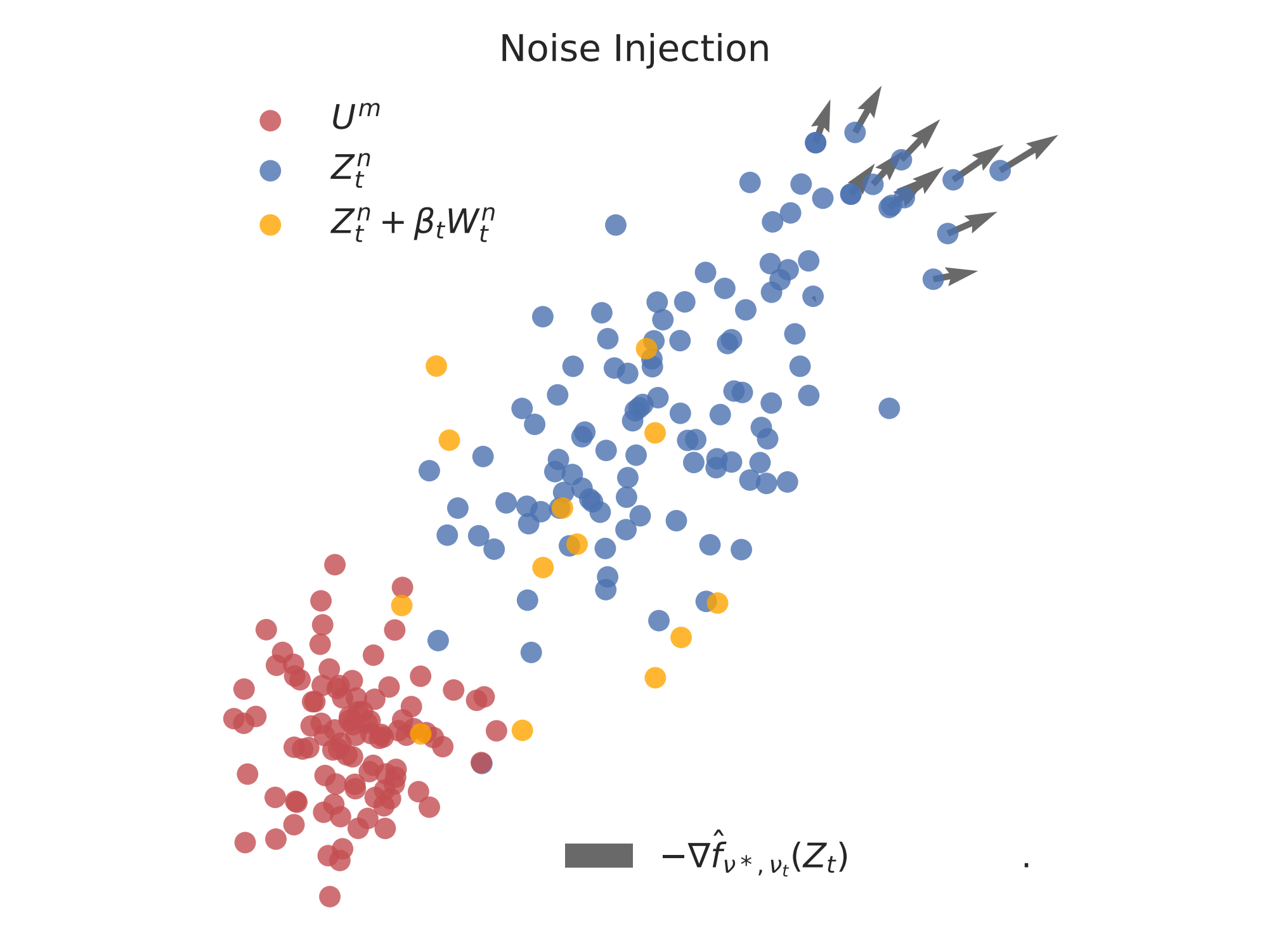
Noise Injection
U^m
Z_t^n
$Z_t^n + \beta_t W_t^n$
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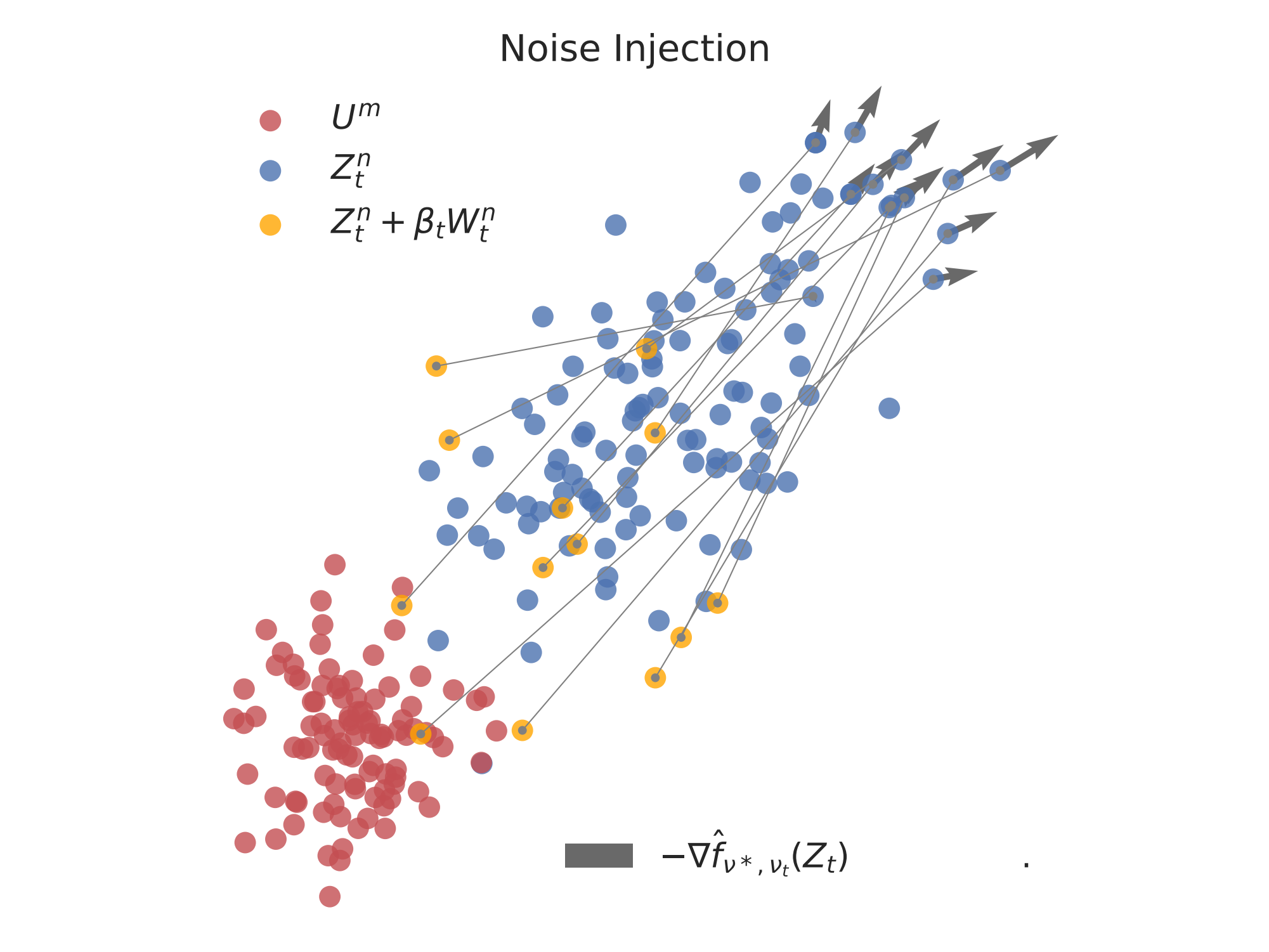
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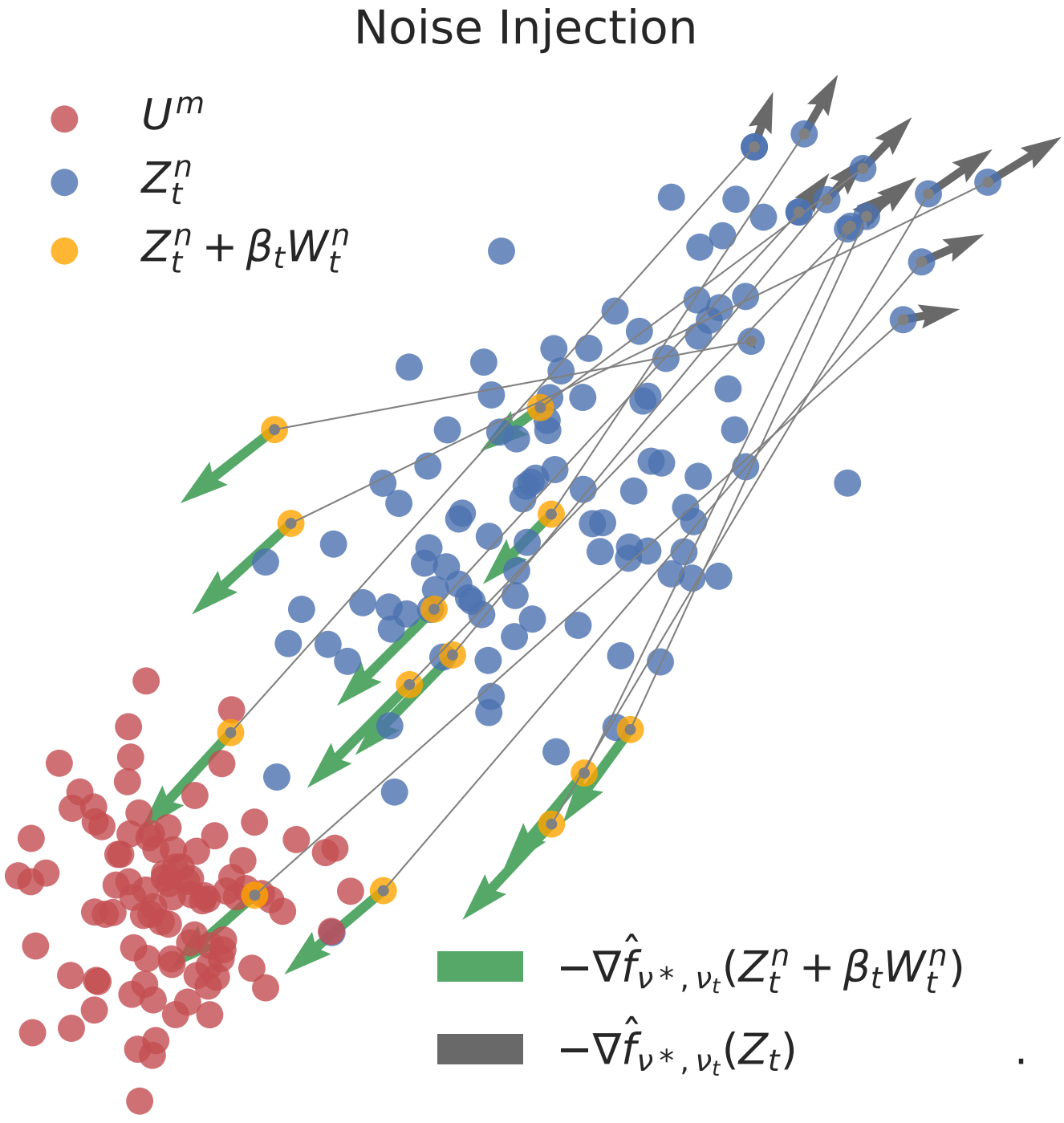
Noise Injection
U^m
Z_t^n
$Z_t^n + \beta_t W_t^n$
$-\nabla \hat{f}_{\nu^*, \nu_t}(Z_t^n + \beta_t W_t^n)$
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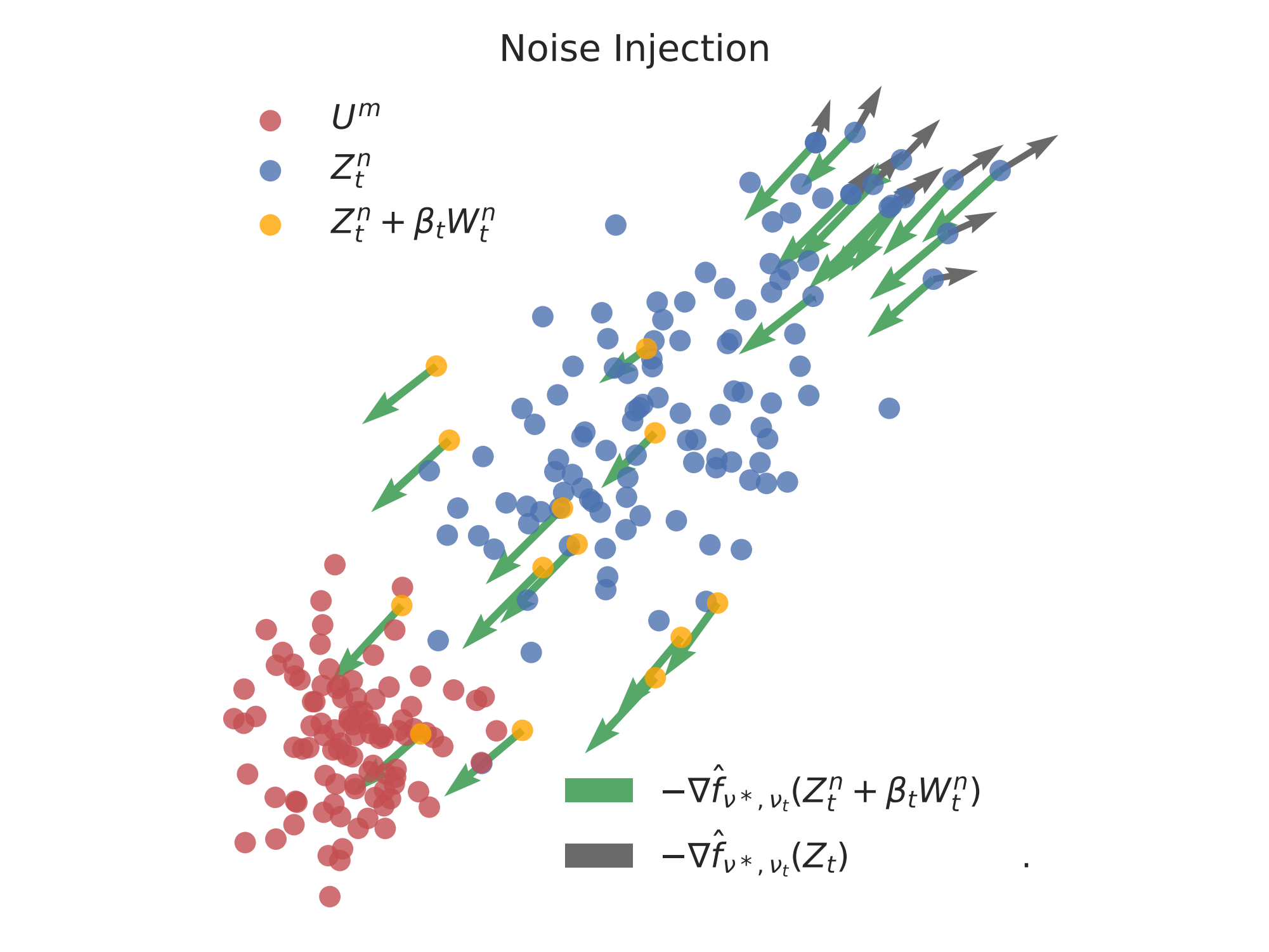
Noise Injection
U^m
Z_t^n
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$-\nabla \hat{f}_{\nu^*, \nu_t}(Z_t^n + \beta_t W_t^n)$
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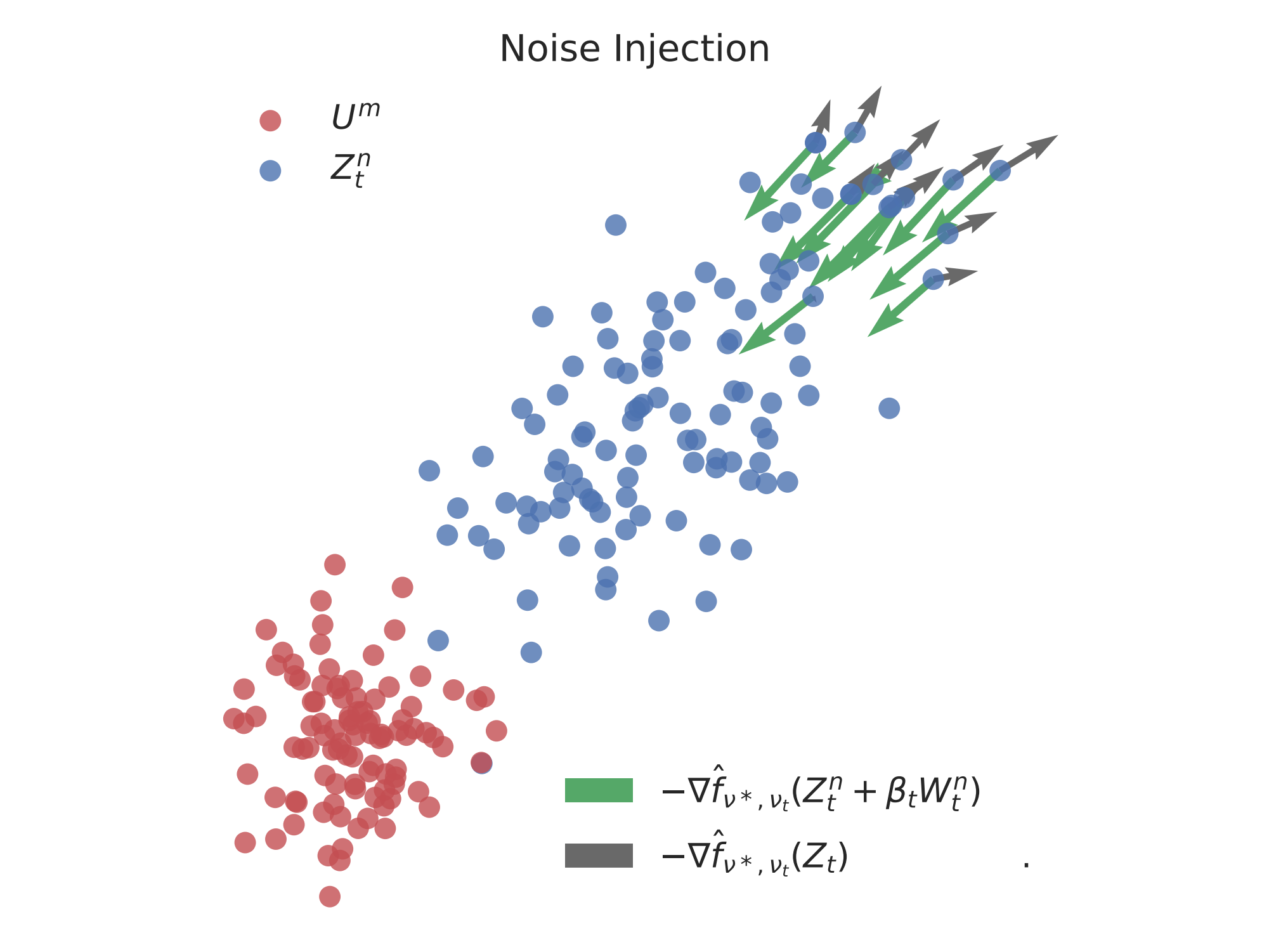
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Z_t^n
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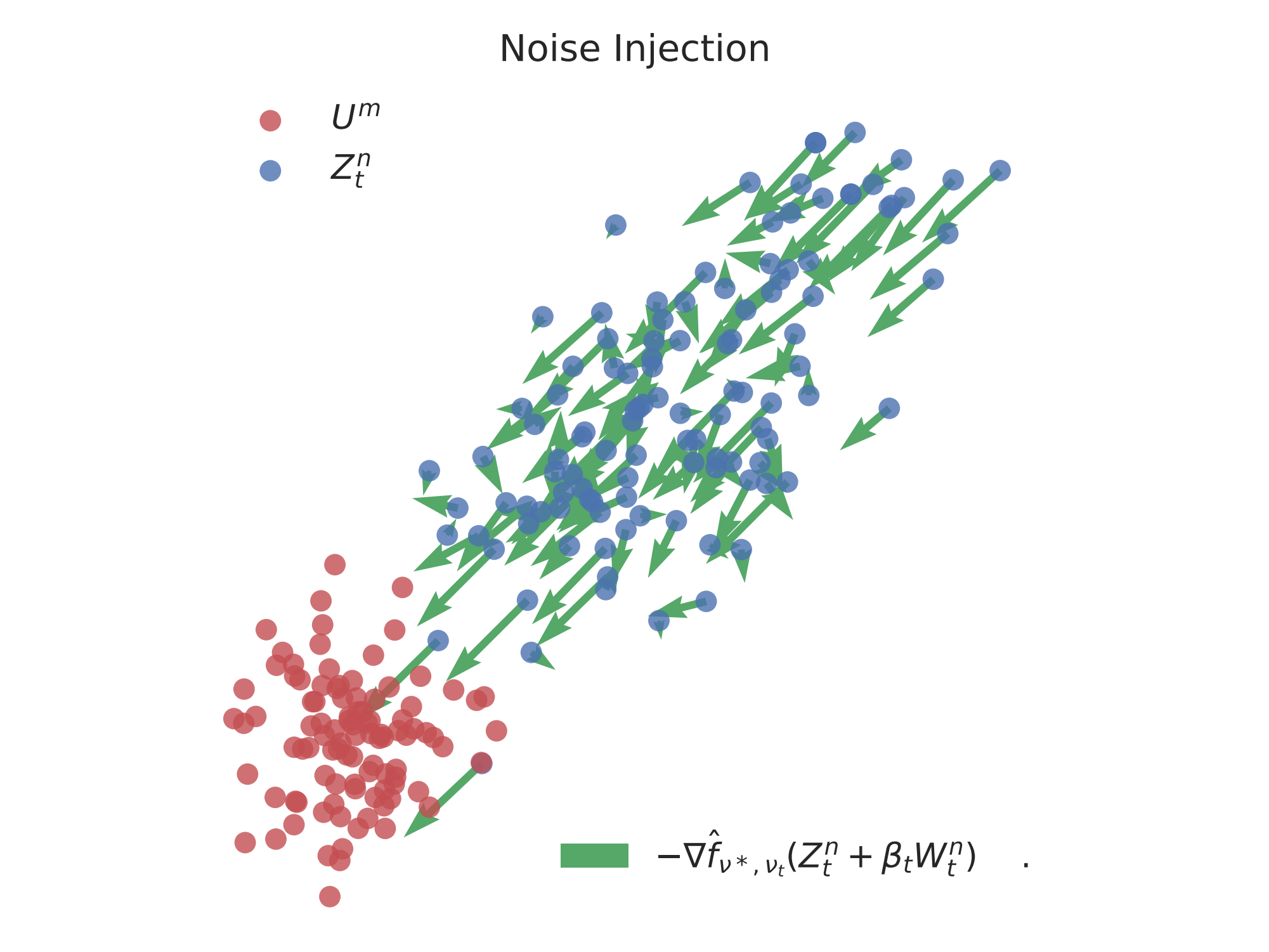
Noise Injection
U^m
Z_t^n
$-\nabla \hat{f}_{\nu^*,\nu_t}(Z_t^n + \beta_t W_t^n)$
.

Noise Injection: Experiments

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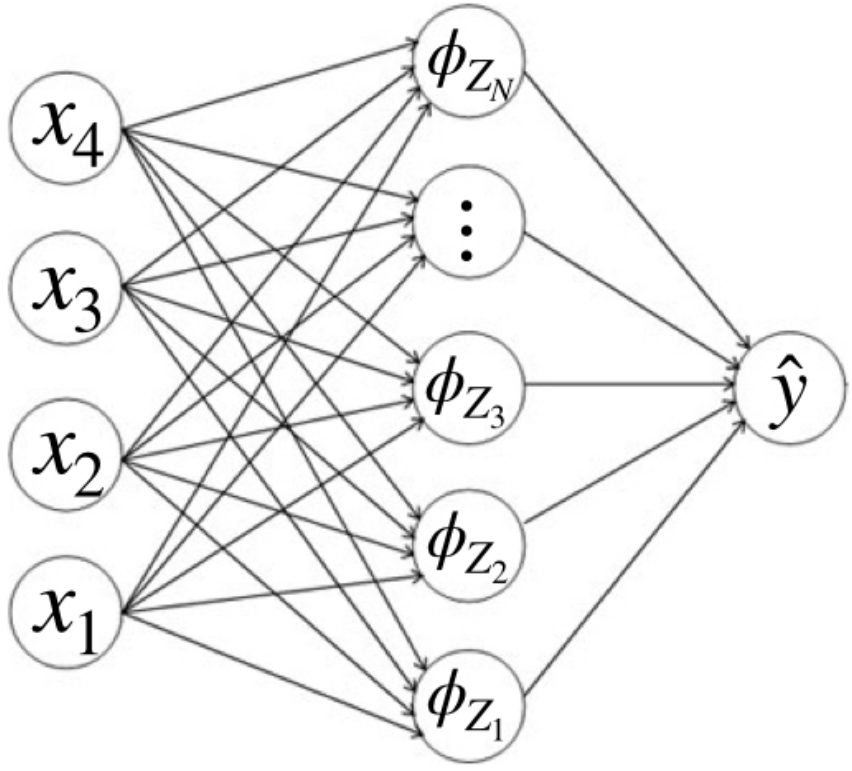
Noise Injection: Experiments

$$(x, y) \sim data$$



$$\min_{Z_1,\ldots,Z_N} \mathbb{E}_{data}[\|\frac{1}{M}\sum_{m}^{M}\phi_{U^m}(x) - \frac{1}{N}\sum_{n=1}^{N}\phi_{Z^n}(x)\|^2]$$

Noise Injection: Experiments

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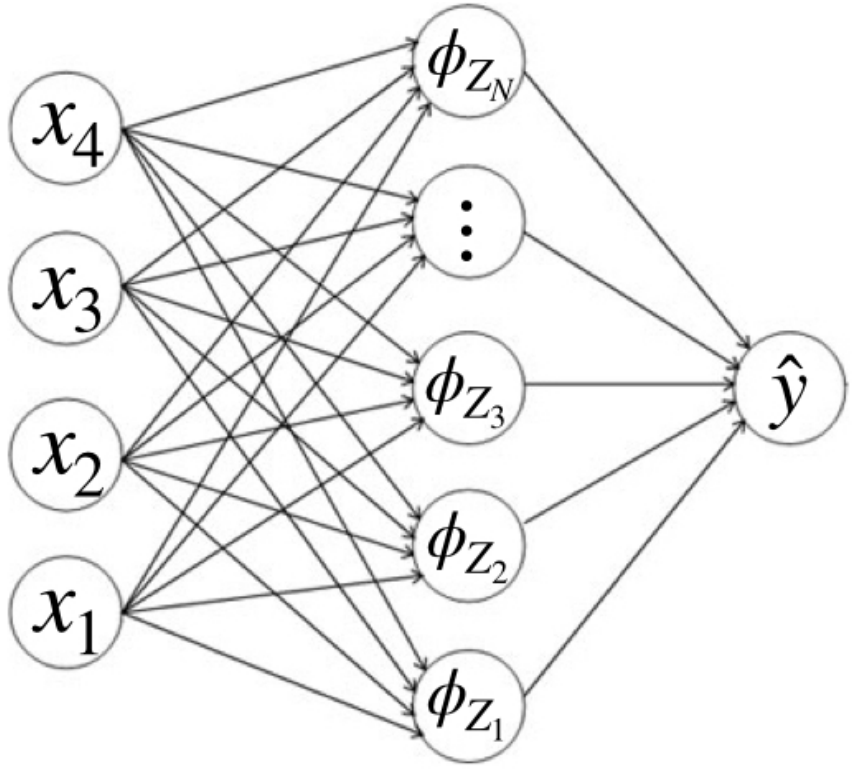
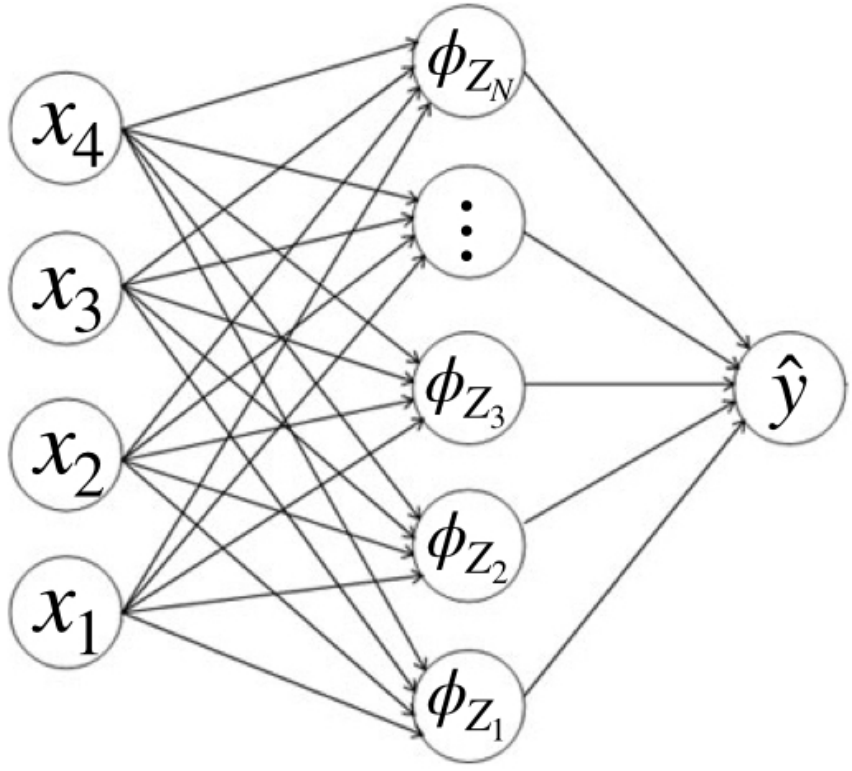


$$\min_{Z_1,\ldots,Z_N} MMD^2(\nu^*, \frac{1}{N}\sum_{n=1}^{N} \delta_{Z^n})$$

$$k(Z, Z') = \mathbb{E}_{data}[\phi_Z(x)\phi_{Z'}(x)]$$

Noise Injection: Experiments

$$(x, y) \sim data$$



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$$\hat{k}(Z, Z') = \frac{1}{B}\sum_{b=1}^{B}\phi_Z(x_b)\phi_{Z'}(x_b)$$

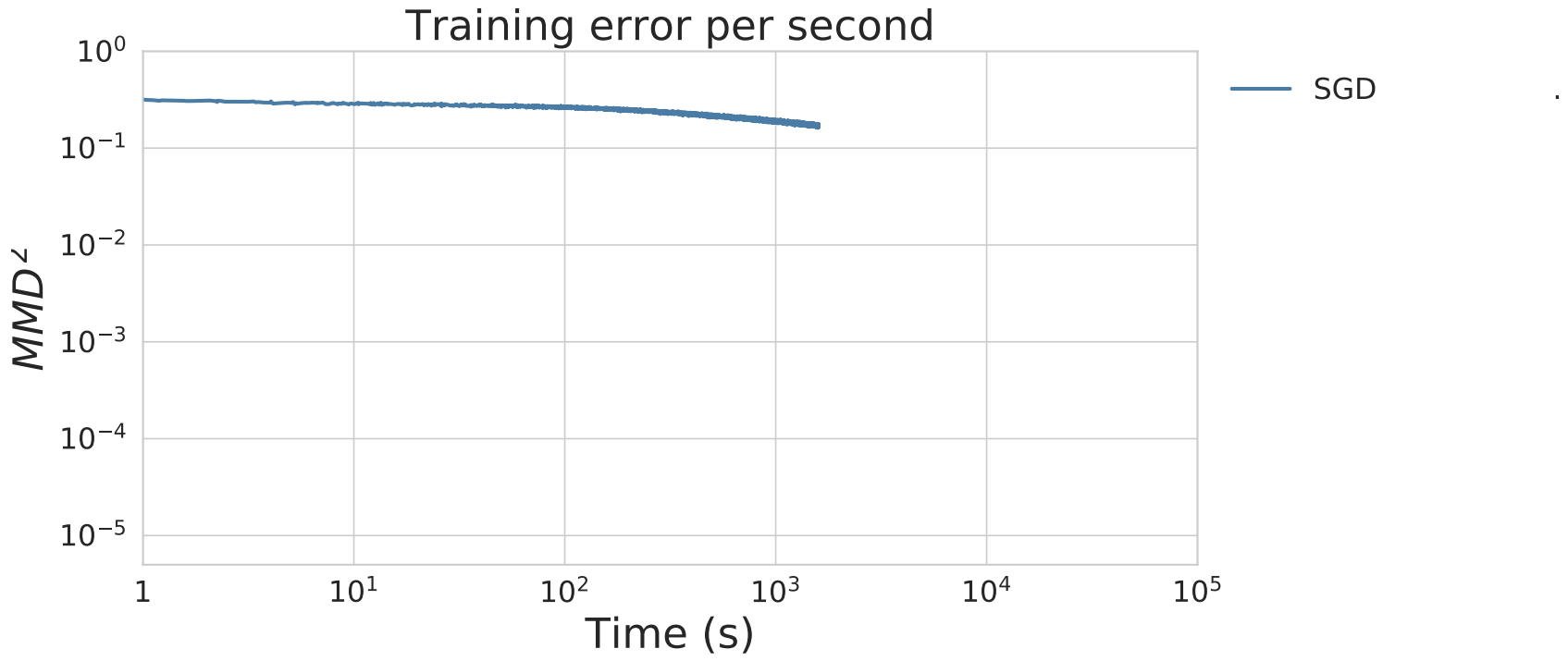
Noise Injection: Experiments

Methods:

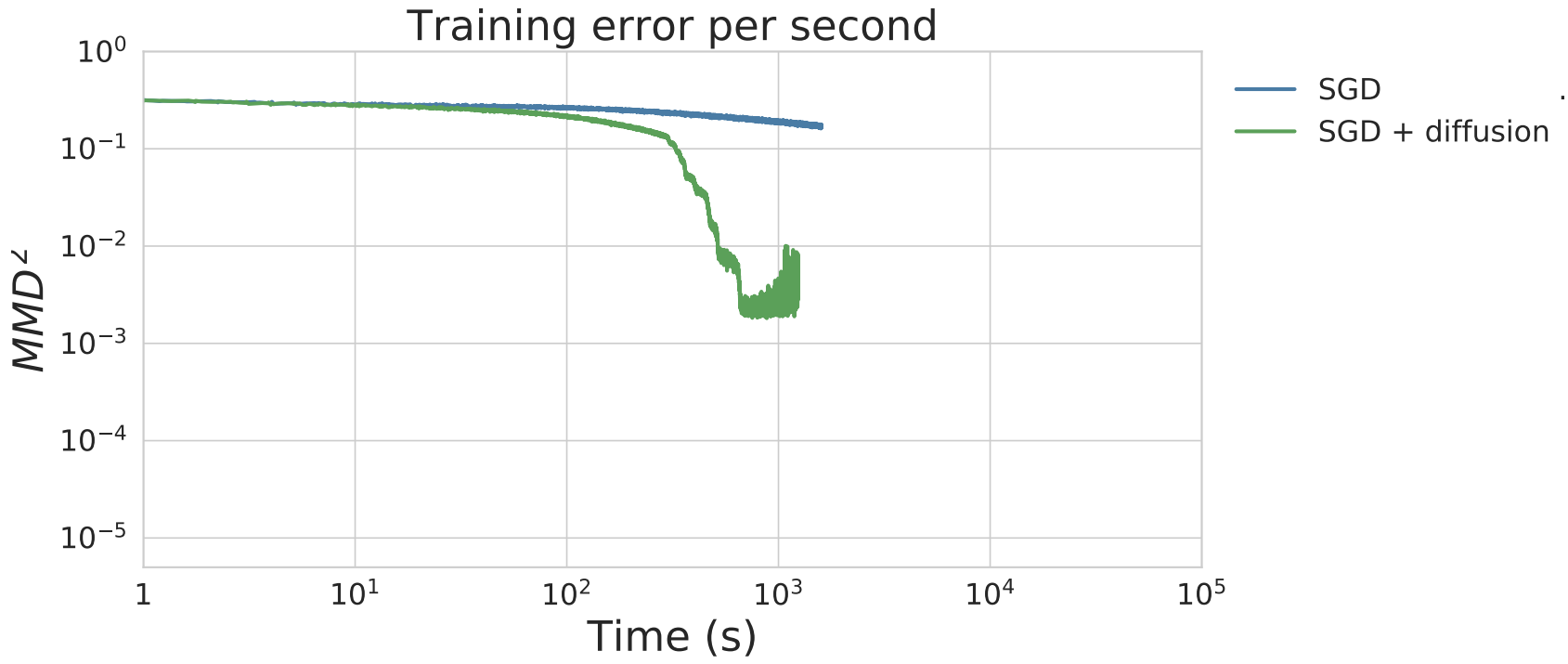
- SGD
- SGD + Noise injection
- SGD + diffusion
- KSD [6]: SGD using the Negative Sobolev distance $\nu \mapsto S(\nu^*|\nu)$ as a loss function: also minimizes the MMD.

[6] [Mroueh et al., 2019]

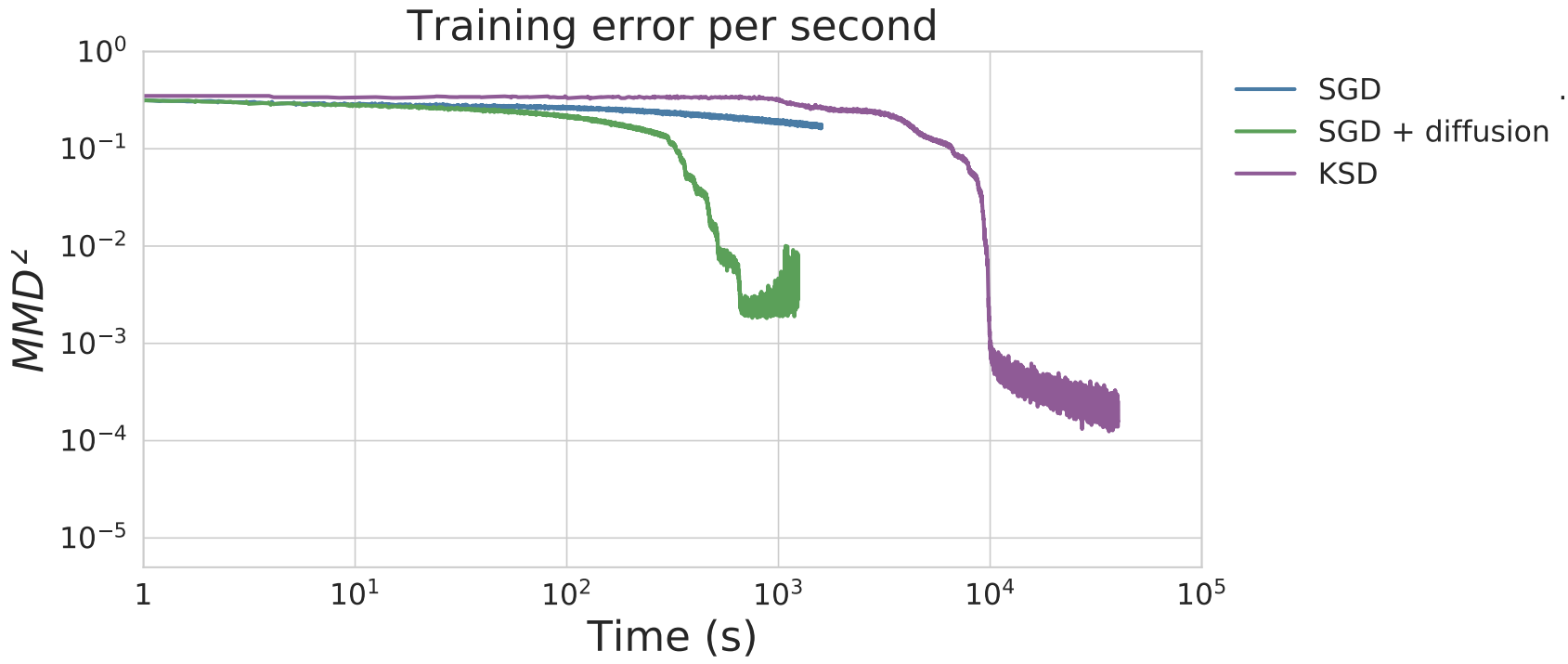
Noise Injection: Experiments



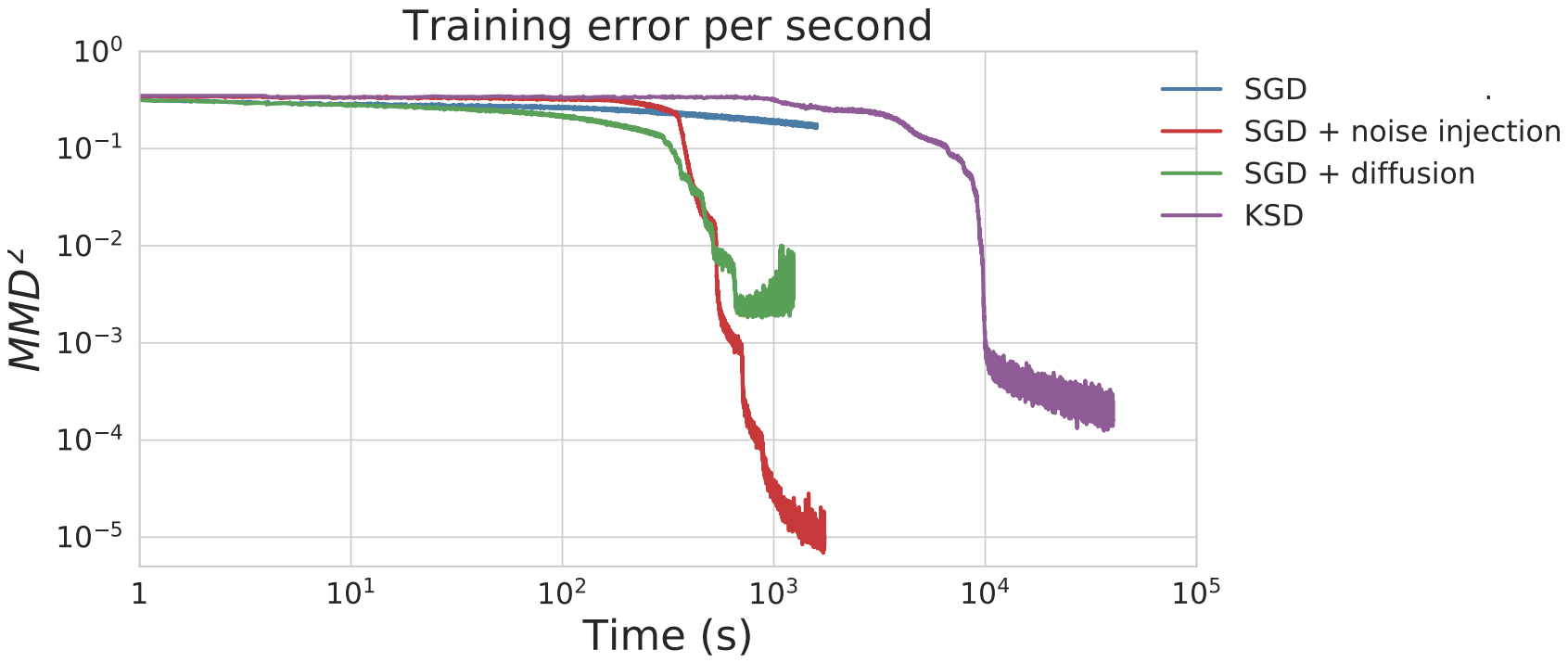
Noise Injection: Experiments



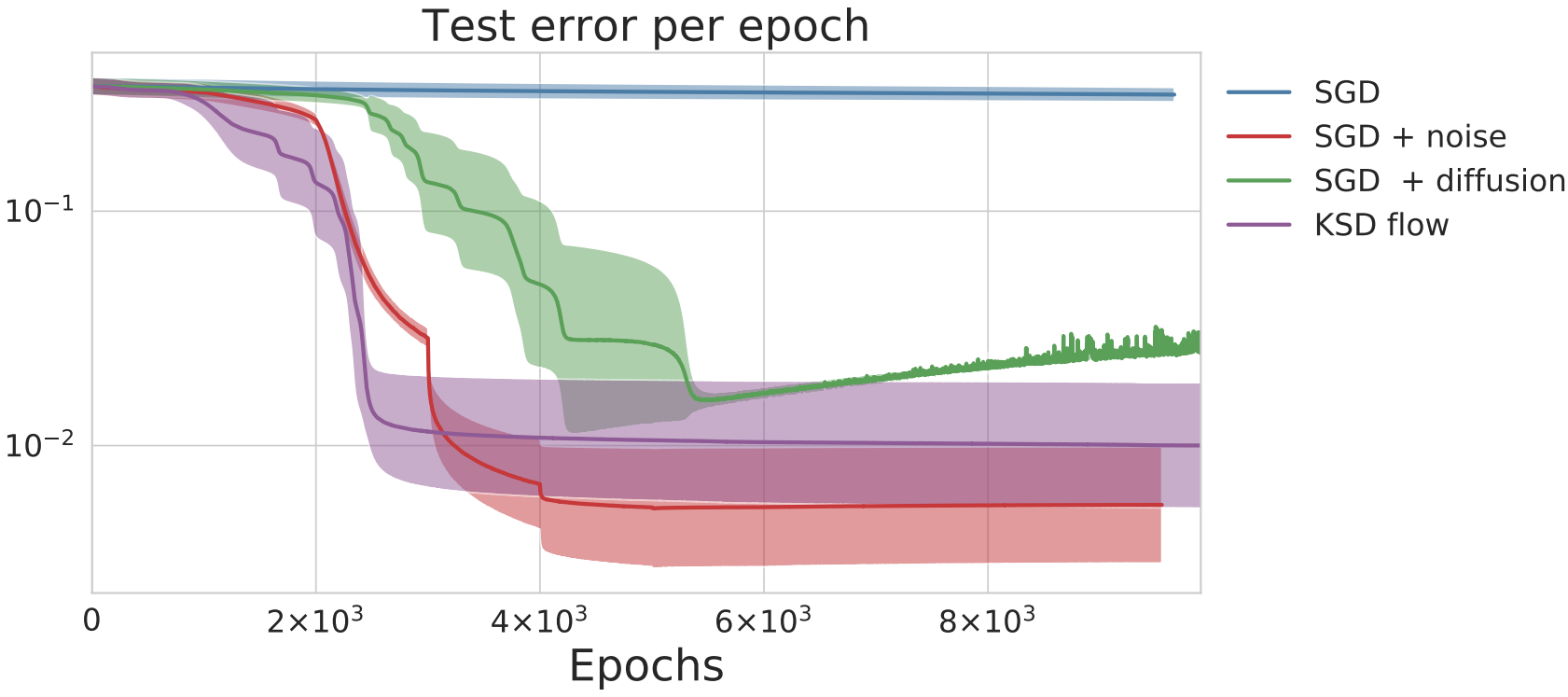
Noise Injection: Experiments



Noise Injection: Experiments



Noise Injection: Experiments



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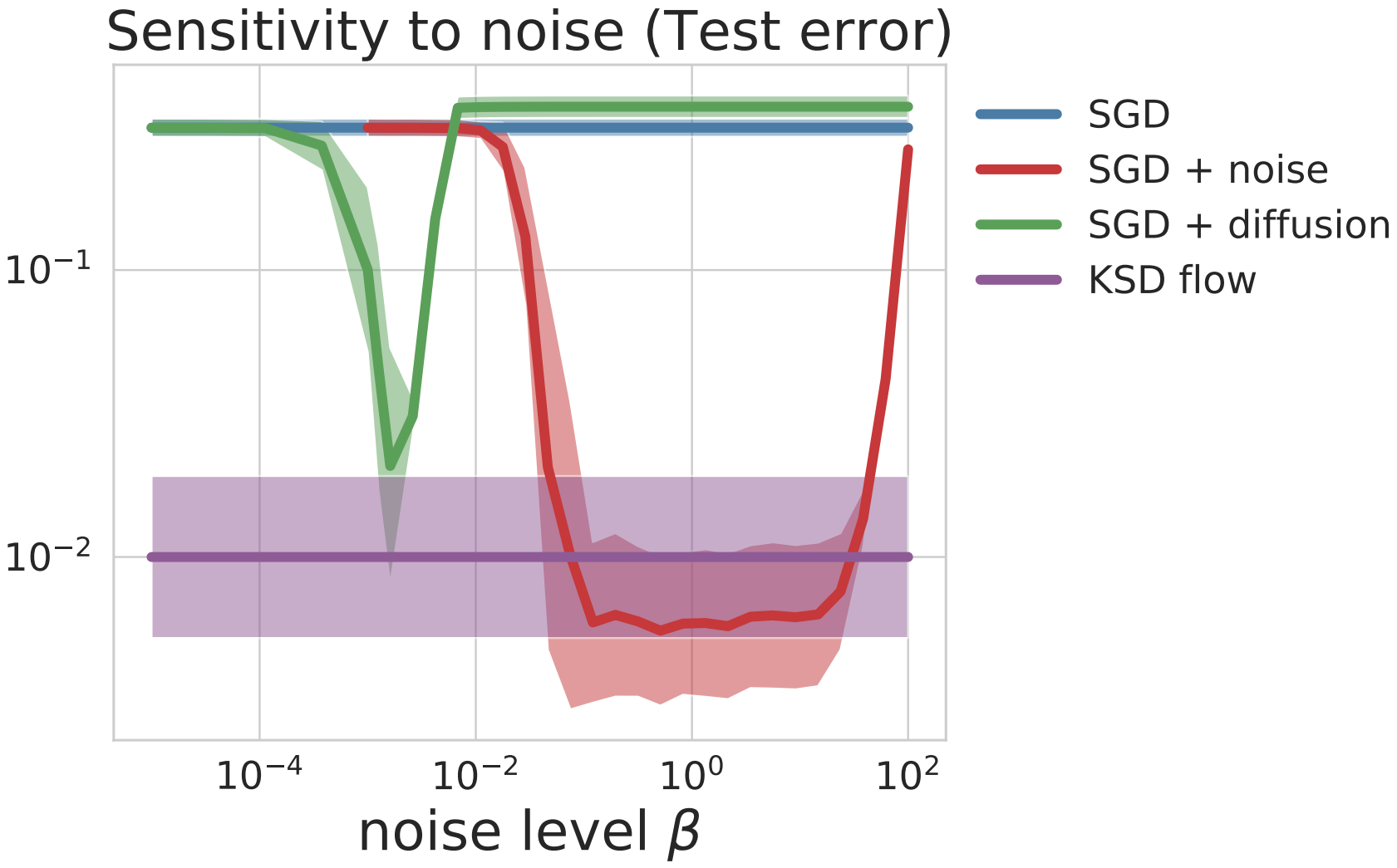

Conclusion

Contributions:

- Provided a convergence criterion for the Wasserstein gradient descent.
- Proposed an extension to the noise injection algorithm for interacting particles and showed it effectiveness on simple examples.

Future work:

- A criterion for convergence that is independent from the whole optimization trajectory.
- Stronger guarantees for the convergence of the noise injection algorithm.

Thank you!

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On the Global Convergence of Gradient Descent for Over-parameterized Models using Optimal Transport.

Gretton, A., Sejdinovic, D., Strathmann, H., Balakrishnan, S., Pontil, M., Fukumizu, K., and Sriperumbudur, B. K. (2012).

Noise Injection: Theory

Tradeoff for β_t

- Large β_t: μ_{t+1} not a descent direction anymore: $MMD^2(\nu^*, \mu_{t+1}) > MMD^2(\nu^*, \mu_t)$

Noise Injection: Theory

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Need β_t such that:

$$MMD^2(\nu^*, \mu_{t+1}) - MMD^2(\nu^*, \mu_t) \leq C\gamma \mathbb{E}_{\substack{X_t \sim \mu_t \\ U_t \sim \mathcal{N}(0,1)}} [\|\nabla f_t(X_t + \beta_t U_t)\|^2]$$

and:

$$\sum_i^t \beta_i^2 \to \infty$$

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Then

$$MMD^2(\nu^*, \nu_t) \leq MMD^2(\nu^*, \nu_0) e^{-C\gamma \sum_i^t \beta_i^2}$$