Conditional Diffusion vs. (Blind) DPS

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Motivation & Problem Statement

Target Task: Conditional image generation for inverse problems (e.g., SEM wafer image restoration).

Core Challenge: Handling Unseen y & Minority Details

- Real-world data (like semiconductor wafers) exhibits severe class imbalance.
- Majority: Normal, smooth surface patterns.
- Minority: High-frequency details (e.g., critical defects).

Question: How do different diffusion frameworks behave when given an *unseen condition* $\mathbf{y}$ containing rare minority details?

Conditional Diffusion: Structural Vulnerability

Li et al., 2022

Mechanism: Condition $\mathbf{y}$ is injected into the U-Net architecture. The network $\epsilon_\theta(\mathbf{x}_t, t, \mathbf{y})$ learns to approximate $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y})$.

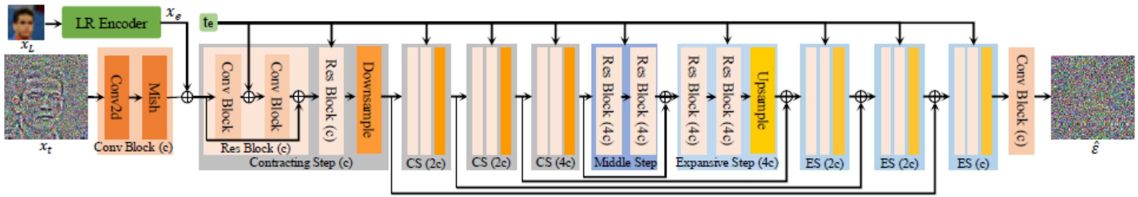

Figure. Score Network Architecture

Vulnerability to Unseen y:

1. **Feature-space Extrapolation:** Unseen $\mathbf{y}$ maps to unexplored regions in the condition embedding space. This might distort attention weights and scale/shift parameters.
2. **Majority Bias:** When uncertain about OOD inputs, the network defaults to the expected loss minimizer (the majority mode).

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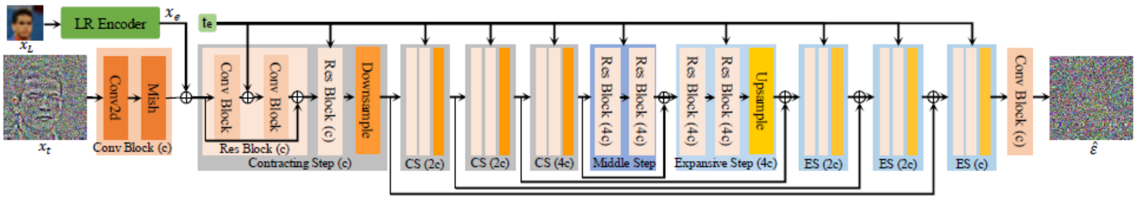

Figure. Score Network Architecture

→**Result:** Minority high-frequency details (defects) are ignored or smoothed out due to the misdirected score vectors.

DPS: Analytic Robustness

Chung, Kim, Mccann, et al., 2023

Mechanism: Uses an unconditional diffusion model and a known forward measurement model ($\mathbf{y} = \mathcal{A}(\mathbf{x}) + \mathbf{n}$).

Score Decomposition (Bayes' Theorem)

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | y) \approx \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t) + \nabla_{\mathbf{x}_t} \log p(\mathbf{y} | \mathbf{x}_t)$$

Robustness to Unseen y:

- The likelihood score $\nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$ is *not learned* but computed analytically via backpropagation through the measurement model.
- The model does not attempt to "interpret" unseen **y** structurally; it merely enforces consistency between the predicted $\hat{\mathbf{x}}_0$ and the observation **y**.

$\rightarrow$ **Result:** Robust to unseen conditions compared to data-driven conditioning.

BlindDPS: Ambiguity in Joint Estimation

Chung, Kim, Kim, and Ye, 2023

Mechanism: Degradation kernel k is unknown. Jointly estimates image $\mathbf{x}$ and kernel k ($\mathbf{y} = k \circledast \mathbf{x} + n$).

Vulnerability to Unseen y (Different from Cond. Diff.):

- **Explain-away Effect:** The unconditional prior $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$ strongly prefers the majority mode (smooth, normal patterns).
- When presented with unseen minority details in $\mathbf{y}$, the joint optimization attributes these anomalies to a distorted kernel k rather than the image $\mathbf{x}$.

$\rightarrow$ **Result:** Rare physical defects are absorbed into the kernel's error space, leading to over-smoothing and loss of crucial details in the restored image $\mathbf{x}$.

SUMMARY

Method	Cause of Failure on Unseen y	Consequence
Conditional Diff.	Structural extrapolation in U-Net	Hallucination, Majority bias
DPS (Known Op.)	(Analytically Robust)	Preserves physics
BlindDPS	$\mathbf{x}$ vs. k parameter ambiguity	Detail loss via kernel distortion

Conclusion for SEM Defect Restoration:

- Relying purely on network-based conditioning is risky for OOD defects.
- Even with BlindDPS, strong physical regularization on the kernel parameter space is strictly required to prevent the prior from erasing minority details.

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