demo_moon

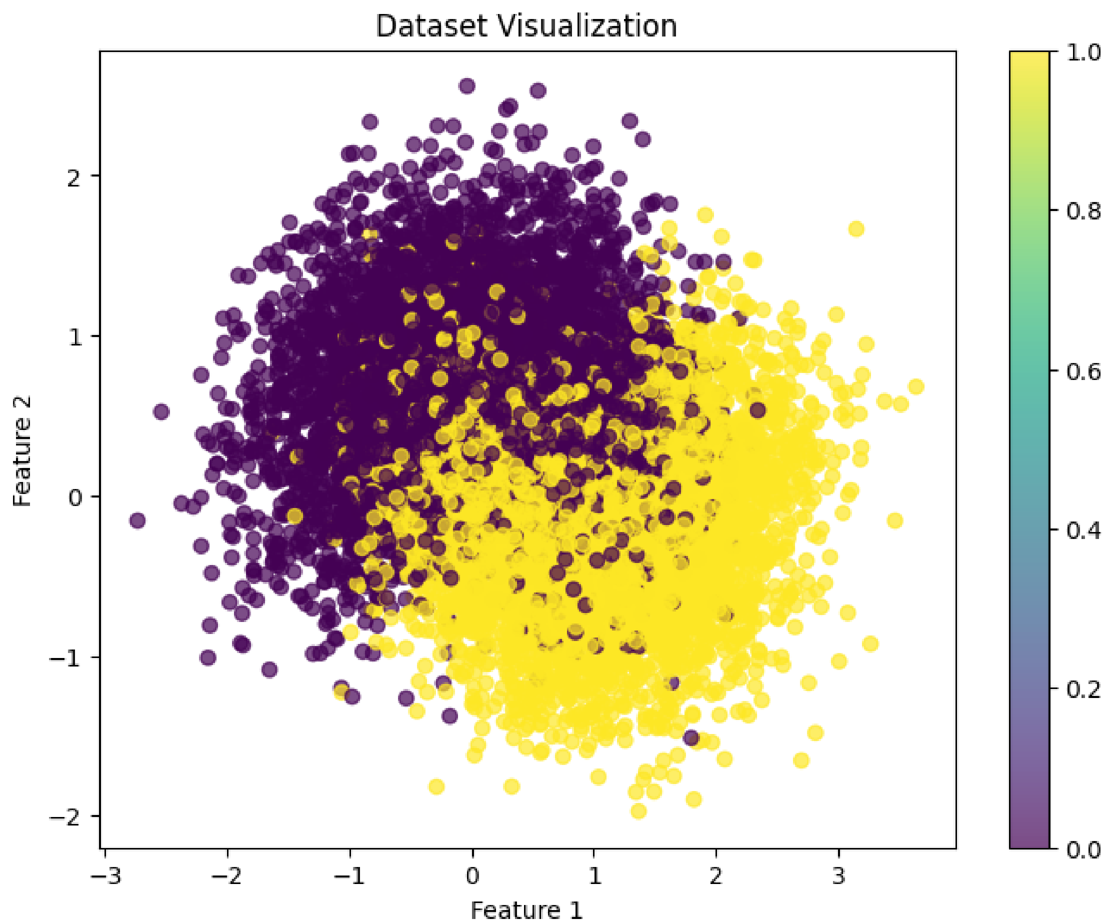
December 4, 2025

[1]:
```
from sklearn.datasets import make_moons
import torch
from torch import nn
from torch.utils.data import DataLoader, TensorDataset
from tqdm import tqdm
import os , sys
sys.path.append(os.path.abspath(os.path.join(os.getcwd(), '..')))
from core.optimization import NSGAConfig, run_nsga
from core.cf_problem import make_cf_problem
from core.data import DataGenerator, DatasetsDG
from core.models import SimpleNN,EnsembleModel
from matplotlib import pyplot as plt
from utils import plot_proba, plot_uncertainty_heatmap, plot_cf_3d
```

[2]:
```
import importlib
import core.optimization
import core.cf_problem

importlib.reload(core.optimization)
importlib.reload(core.cf_problem)
```

[2]:
```
<module 'core.cf_problem' from 'e:\\Thieses mit
Thies\\uamocf\\core\\cf_problem.py'>
```

[3]:
```
ds=make_moons(n_samples=10000, noise=0.5, random_state=42)

tds = TensorDataset(torch.tensor(ds[0], dtype=torch.float32), torch.
 ↪tensor(ds[1], dtype=torch.long))
dg=DatasetsDG(tds, num_classes=2)
dg.plot()
```



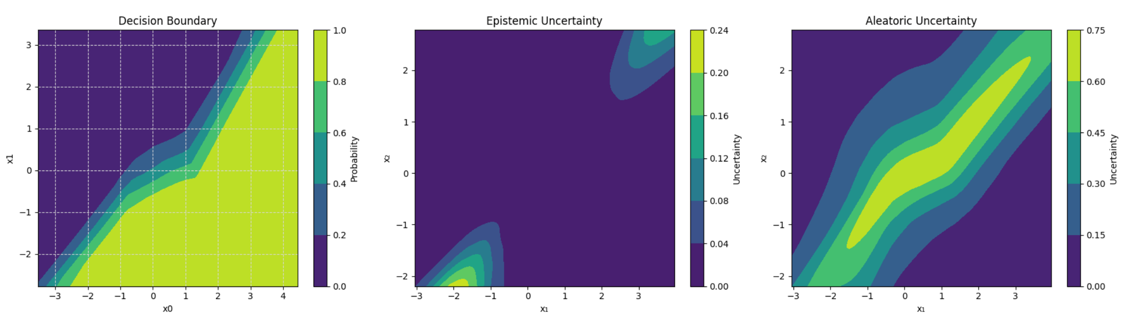

```
[4]: models = [SimpleNN(input_dim=2, hidden_dim=14, output_dim=2, depth=3) for _ in␣
     ↪range(5)]
     ensemble_model = EnsembleModel(models=models)


     # train each model in the ensemble
     device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
     ensemble_model.to(device)
     epochs = 150
     val_data = dg.sample(500, seed=123)
     for model in ensemble_model.models:
         seed = 42 + hash(model) % 1000  # Simple way to get different seeds
         samples = dg.sample(400, seed=seed)
         _tds= TensorDataset(samples[0].to(device), samples[1].to(device))
         DL=DataLoader(_tds, batch_size=256, shuffle=True)
         model.train()
```

```python
    bar = tqdm(range(epochs), desc="Training Model", colour="blue",␣
↪unit="epoch")
    running_loss = 0.0
    optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
    criterion = nn.CrossEntropyLoss()
    for epoch in bar:
        for inputs, labels in DL:
            optimizer.zero_grad()
            outputs = model(inputs)
            loss = criterion(outputs, labels)
            loss.backward()
            optimizer.step()
            running_loss += loss.item()
        bar.set_postfix({"loss": running_loss / (epoch + 1)})

    model.eval()
    with torch.no_grad():
        val_inputs, val_labels = val_data[0].to(device), val_data[1].to(device)
        val_outputs = model(val_inputs)
        _, val_preds = torch.max(val_outputs, 1)
        _, val_labels_idx = torch.max(val_labels, 1)
        val_accuracy = (val_preds == val_labels_idx).float().mean().item()
        print(f"Validation Accuracy: {val_accuracy * 100:.2f}%")
    print(f"Finished Training Model")
```

```
Training Model: 100%|      | 150/150 [00:02<00:00, 50.07epoch/s,
loss=0.94]

Validation Accuracy: 80.20%
Finished Training Model

Training Model: 100%|      | 150/150 [00:01<00:00, 120.15epoch/s,
loss=0.933]

Validation Accuracy: 80.80%
Finished Training Model

Training Model: 100%|      | 150/150 [00:01<00:00, 113.39epoch/s,
loss=0.92]

Validation Accuracy: 79.80%
Finished Training Model

Training Model: 100%|      | 150/150 [00:01<00:00, 115.33epoch/s,
loss=0.955]

Validation Accuracy: 80.40%
Finished Training Model

Training Model: 100%|      | 150/150 [00:01<00:00, 117.83epoch/s,
loss=0.975]
```

```
Validation Accuracy: 79.40%
Finished Training Model
```

[5]:
```python
# plot decision boundary


fig, axes = plt.subplots(1, 3, figsize=(18, 5))

plot_proba(ensemble_model.models[0], ds[0], levels=5, ax=axes[0])
axes[0].set_title("Decision Boundary")

plot_uncertainty_heatmap(ensemble_model, ds[0], uncertainty_type="epistemic", device=device, levels=5, ax=axes[1])
axes[1].set_title("Epistemic Uncertainty")

plot_uncertainty_heatmap(ensemble_model, ds[0], uncertainty_type="aleatoric", device=device, levels=5, ax=axes[2])
axes[2].set_title("Aleatoric Uncertainty")

plt.tight_layout()
plt.show()
```



[6]:
```python
x_factual = torch.tensor([[2, -1]], dtype=torch.float32)
y_target = torch.tensor([0], dtype=torch.long)
X_obs = dg.sample(1000, seed=456)[0]
if isinstance(X_obs, torch.Tensor):
    X_obs = X_obs.clone().detach().float()
else:
    X_obs = torch.tensor(X_obs, dtype=torch.float32)

NSGA2_config = NSGAConfig(
    pop_size=150,
    min_gen=250,
    max_gen=5950,
```

```
    use_conditional_mutator=True,
    conditional_mutator_prob=0.7,
    use_reset_operator=True,
    reset_prob=0.05,
)

# ============ VERSION 1: With Uncertainty (EU/AU) ============
print("=" * 50)
print("Running VERSION 1: With Epistemic & Aleatoric Uncertainty")
print("Objectives: [Validity, EU, Sparsity, -AU]")
print("=" * 50)
problem_uncertainty = make_cf_problem(
    ensemble_model.models[0], x_factual, y_target, X_obs,
    device=device,
    ensemble=ensemble_model  # Enables EU/AU objectives
)
results_uncertainty = run_nsga(problem_uncertainty, NSGA2_config, X_obs=X_obs.
 ↪numpy(), x_factual=x_factual.numpy())

# ============ VERSION 2: Simple (Similarity/Plausibility) ============
print("\n" + "=" * 50)
print("Running VERSION 2: Simple (Similarity & Plausibility)")
print("Objectives: [Validity, Similarity, Sparsity, Plausibility]")
print("=" * 50)
problem_simple = make_cf_problem(
    ensemble_model.models[0], x_factual, y_target, X_obs,
    device=device,
    ensemble=None  # No ensemble = uses Similarity/Plausibility objectives
)
results_simple = run_nsga(problem_simple, NSGA2_config, X_obs=X_obs.numpy(),␣
 ↪x_factual=x_factual.numpy())

print("\n Both optimizations completed!")
```

```
==================================================
Running VERSION 1: With Epistemic & Aleatoric Uncertainty
Objectives: [Validity, EU, Sparsity, -AU]
==================================================
Gen    1 | Valid CFs (pop):  66 | Pareto front:  48 | Best P(target): 0.994 |
Mean Sparsity: 1.979
Gen   10 | Valid CFs (pop): 124 | Pareto front: 150 | Best P(target): 0.993 |
Mean Sparsity: 1.773
Gen   20 | Valid CFs (pop): 128 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.787
Gen   30 | Valid CFs (pop): 132 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.800
Gen   40 | Valid CFs (pop): 124 | Pareto front: 150 | Best P(target): 0.994 |
```

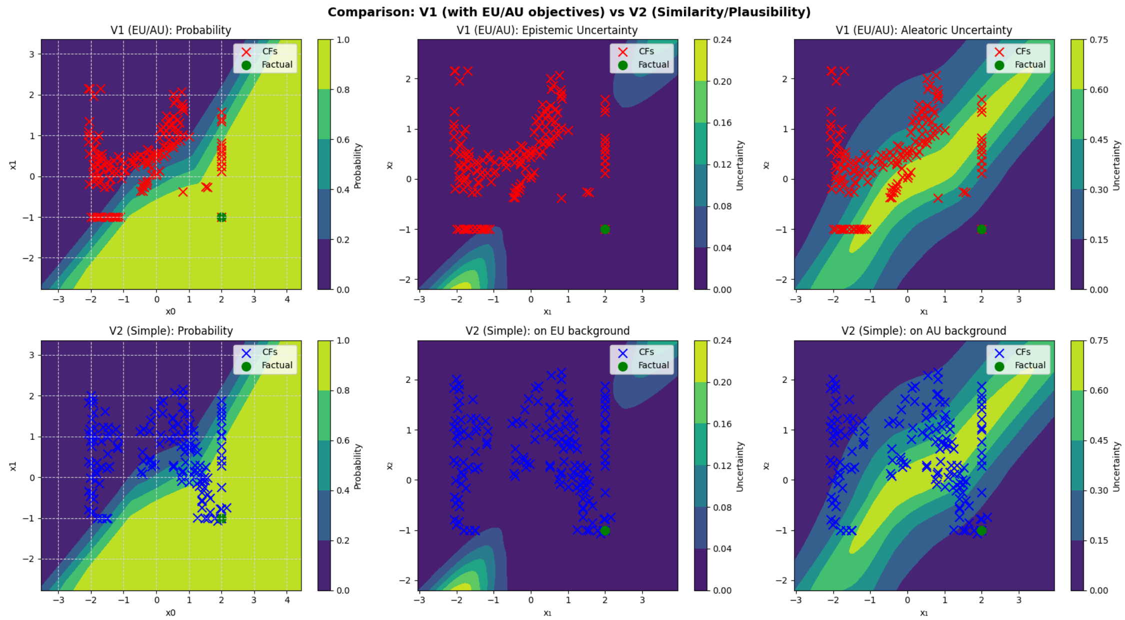
```
Mean Sparsity: 1.793
Gen  50 | Valid CFs (pop): 129 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.807
Gen  60 | Valid CFs (pop): 132 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.787
Gen  70 | Valid CFs (pop): 130 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.807
Gen  80 | Valid CFs (pop): 127 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.767
Gen  90 | Valid CFs (pop): 128 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.773
Gen 100 | Valid CFs (pop): 126 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.767
Gen 110 | Valid CFs (pop): 130 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.787
Gen 120 | Valid CFs (pop): 127 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.767
Gen 130 | Valid CFs (pop): 127 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.793
Gen 140 | Valid CFs (pop): 130 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.807
Gen 150 | Valid CFs (pop): 131 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.780
Gen 160 | Valid CFs (pop): 130 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.787
Gen 170 | Valid CFs (pop): 128 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.780
Gen 180 | Valid CFs (pop): 125 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.760
Gen 190 | Valid CFs (pop): 132 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.813
Gen 200 | Valid CFs (pop): 124 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.720
Gen 210 | Valid CFs (pop): 132 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.787
Gen 220 | Valid CFs (pop): 126 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.753
Gen 230 | Valid CFs (pop): 130 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.833
Gen 240 | Valid CFs (pop): 130 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.813
Gen 250 | Valid CFs (pop): 129 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.813

==================================================
Running VERSION 2: Simple (Similarity & Plausibility)
Objectives: [Validity, Similarity, Sparsity, Plausibility]
==================================================
```

```
Gen    1 | Valid CFs (pop):  66 | Pareto front:  62 | Best P(target): 0.994 |
Mean Sparsity: 1.984
Gen   10 | Valid CFs (pop): 107 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.853
Gen   20 | Valid CFs (pop):  99 | Pareto front: 150 | Best P(target): 0.993 |
Mean Sparsity: 1.853
Gen   30 | Valid CFs (pop): 110 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.867
Gen   40 | Valid CFs (pop): 105 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.840
Gen   50 | Valid CFs (pop): 105 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.873
Gen   60 | Valid CFs (pop): 104 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.833
Gen   70 | Valid CFs (pop): 102 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.833
Gen   80 | Valid CFs (pop): 111 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.873
Gen   90 | Valid CFs (pop): 114 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.847
Gen  100 | Valid CFs (pop): 104 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.867
Gen  110 | Valid CFs (pop): 106 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.860
Gen  120 | Valid CFs (pop):  98 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.807
Gen  130 | Valid CFs (pop): 104 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.847
Gen  140 | Valid CFs (pop): 104 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.813
Gen  150 | Valid CFs (pop): 106 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.847
Gen  160 | Valid CFs (pop): 103 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.833
Gen  170 | Valid CFs (pop): 103 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.853
Gen  180 | Valid CFs (pop): 105 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.847
Gen  190 | Valid CFs (pop): 114 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.887
Gen  200 | Valid CFs (pop): 107 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.787
Gen  210 | Valid CFs (pop): 112 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.833
Gen  220 | Valid CFs (pop): 101 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.847
Gen  230 | Valid CFs (pop): 106 | Pareto front: 150 | Best P(target): 0.995 |
Mean Sparsity: 1.840
```

```
Gen  240 | Valid CFs (pop): 108 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.867
Gen  250 | Valid CFs (pop): 103 | Pareto front: 150 | Best P(target): 0.994 |
Mean Sparsity: 1.840

 Both optimizations completed!
```

[7]:
```
# Compare both versions in 2D feature space
fig, axes = plt.subplots(2, 3, figsize=(18, 10))

cf_uncertainty = torch.tensor(results_uncertainty.X, dtype=torch.float32).cpu().
 ↪numpy()
cf_simple = torch.tensor(results_simple.X, dtype=torch.float32).cpu().numpy()

# ============ ROW 1: VERSION 1 - With Uncertainty (EU/AU) ============
# 1. Probability background
plot_proba(ensemble_model.models[0], ds[0], levels=5, ax=axes[0, 0])
axes[0, 0].scatter(cf_uncertainty[:, 0], cf_uncertainty[:, 1], color='red',␣
 ↪marker='x', s=100, label='CFs')
axes[0, 0].scatter(x_factual[0, 0].item(), x_factual[0, 1].item(),␣
 ↪color='green', marker='o', s=100, label='Factual')
axes[0, 0].set_title("V1 (EU/AU): Probability")
axes[0, 0].legend()

# 2. Epistemic Uncertainty background
plot_uncertainty_heatmap(ensemble_model, ds[0], device=device,␣
 ↪uncertainty_type="epistemic", levels=5, ax=axes[0, 1])
axes[0, 1].scatter(cf_uncertainty[:, 0], cf_uncertainty[:, 1], color='red',␣
 ↪marker='x', s=100, label='CFs')
axes[0, 1].scatter(x_factual[0, 0].item(), x_factual[0, 1].item(),␣
 ↪color='green', marker='o', s=100, label='Factual')
axes[0, 1].set_title("V1 (EU/AU): Epistemic Uncertainty")
axes[0, 1].legend()

# 3. Aleatoric Uncertainty background
plot_uncertainty_heatmap(ensemble_model, ds[0], device=device,␣
 ↪uncertainty_type="aleatoric", levels=5, ax=axes[0, 2])
axes[0, 2].scatter(cf_uncertainty[:, 0], cf_uncertainty[:, 1], color='red',␣
 ↪marker='x', s=100, label='CFs')
axes[0, 2].scatter(x_factual[0, 0].item(), x_factual[0, 1].item(),␣
 ↪color='green', marker='o', s=100, label='Factual')
axes[0, 2].set_title("V1 (EU/AU): Aleatoric Uncertainty")
axes[0, 2].legend()

# ============ ROW 2: VERSION 2 - Simple (Similarity/Plausibility) ============
# 1. Probability background
plot_proba(ensemble_model.models[0], ds[0], levels=5, ax=axes[1, 0])
```

```
axes[1, 0].scatter(cf_simple[:, 0], cf_simple[:, 1], color='blue', marker='x',␣
↪s=100, label='CFs')
axes[1, 0].scatter(x_factual[0, 0].item(), x_factual[0, 1].item(),␣
↪color='green', marker='o', s=100, label='Factual')
axes[1, 0].set_title("V2 (Simple): Probability")
axes[1, 0].legend()

# 2. Epistemic Uncertainty background (for comparison)
plot_uncertainty_heatmap(ensemble_model, ds[0], device=device,␣
↪uncertainty_type="epistemic", levels=5, ax=axes[1, 1])
axes[1, 1].scatter(cf_simple[:, 0], cf_simple[:, 1], color='blue', marker='x',␣
↪s=100, label='CFs')
axes[1, 1].scatter(x_factual[0, 0].item(), x_factual[0, 1].item(),␣
↪color='green', marker='o', s=100, label='Factual')
axes[1, 1].set_title("V2 (Simple): on EU background")
axes[1, 1].legend()

# 3. Aleatoric Uncertainty background (for comparison)
plot_uncertainty_heatmap(ensemble_model, ds[0], device=device,␣
↪uncertainty_type="aleatoric", levels=5, ax=axes[1, 2])
axes[1, 2].scatter(cf_simple[:, 0], cf_simple[:, 1], color='blue', marker='x',␣
↪s=100, label='CFs')
axes[1, 2].scatter(x_factual[0, 0].item(), x_factual[0, 1].item(),␣
↪color='green', marker='o', s=100, label='Factual')
axes[1, 2].set_title("V2 (Simple): on AU background")
axes[1, 2].legend()

plt.suptitle("Comparison: V1 (with EU/AU objectives) vs V2 (Similarity/
↪Plausibility)", fontsize=14, fontweight='bold')
plt.tight_layout()
plt.show()
```



[8]:
```python
import importlib
import utils
importlib.reload(utils)
from utils import plot_cf_3d

# Convert tensors to numpy arrays for the plot
x_factual_np = x_factual.cpu().numpy() if isinstance(x_factual, torch.Tensor) else x_factual
context_data = dg.sample(10000, seed=789)[0]
context_np = context_data.cpu().numpy() if isinstance(context_data, torch.Tensor) else context_data

# ============ 3D Objective Space: VERSION 1 (EU/AU) ============
print("=" * 50)
print("3D Objective Space: VERSION 1 (with EU/AU)")
print("Axes: EU (x), Validity (y), AU (z - reversed)")
print("=" * 50)
plot_cf_3d(results=results_uncertainty, x_factual=x_factual_np, context=context_np)
```

```
==================================================
3D Objective Space: VERSION 1 (with EU/AU)
Axes: EU (x), Validity (y), AU (z - reversed)
==================================================
```

[9]:
```python
# ============ 3D Objective Space: VERSION 2 (Simple) ============
print("=" * 50)
```

```python
print("3D Objective Space: VERSION 2 (Similarity/Plausibility)")
print("Axes: Similarity (x), Validity (y), Plausibility (z)")
print("=" * 50)
plot_cf_3d(results=results_simple, x_factual=x_factual_np, context=context_np)
```

```
==================================================
3D Objective Space: VERSION 2 (Similarity/Plausibility)
Axes: Similarity (x), Validity (y), Plausibility (z)
==================================================
```

[10]:

```python
# ============ Summary Comparison ============
print("=" * 60)
print("SUMMARY: Objective Values Comparison")
print("=" * 60)

print("\n--- VERSION 1: With Uncertainty (EU/AU) ---")
print("Objectives: [Validity, Epistemic U., Sparsity, -Aleatoric U.]")
print(f"Number of Pareto solutions: {len(results_uncertainty.X)}")
print(f"Validity range: [{results_uncertainty.F[:,0].min():.4f},␣
↪{results_uncertainty.F[:,0].max():.4f}]")
print(f"Epistemic U. range: [{results_uncertainty.F[:,1].min():.4f},␣
↪{results_uncertainty.F[:,1].max():.4f}]")
print(f"Sparsity range: [{results_uncertainty.F[:,2].min():.4f},␣
↪{results_uncertainty.F[:,2].max():.4f}]")
print(f"-AU range: [{results_uncertainty.F[:,3].min():.4f},␣
↪{results_uncertainty.F[:,3].max():.4f}]")
print(f" → AU (positive): [{-results_uncertainty.F[:,3].max():.4f},␣
↪{-results_uncertainty.F[:,3].min():.4f}]")

print("\n--- VERSION 2: Simple (Similarity/Plausibility) ---")
print("Objectives: [Validity, Similarity, Sparsity, Plausibility]")
print(f"Number of Pareto solutions: {len(results_simple.X)}")
print(f"Validity range: [{results_simple.F[:,0].min():.4f}, {results_simple.F[:
↪,0].max():.4f}]")
print(f"Similarity range: [{results_simple.F[:,1].min():.4f}, {results_simple.
↪F[:,1].max():.4f}]")
print(f"Sparsity range: [{results_simple.F[:,2].min():.4f}, {results_simple.F[:
↪,2].max():.4f}]")
print(f"Plausibility range: [{results_simple.F[:,3].min():.4f}, {results_simple.
↪F[:,3].max():.4f}]")
```

```
============================================================
SUMMARY: Objective Values Comparison
============================================================

--- VERSION 1: With Uncertainty (EU/AU) ---
Objectives: [Validity, Epistemic U., Sparsity, -Aleatoric U.]
Number of Pareto solutions: 150
```

```
Validity range: [0.0048, 0.9890]
Epistemic U. range: [0.0001, 0.0426]
Sparsity range: [0.0000, 2.0000]
-AU range: [-0.6926, -0.0487]
 → AU (positive): [0.0487, 0.6926]

--- VERSION 2: Simple (Similarity/Plausibility) ---
Objectives: [Validity, Similarity, Sparsity, Plausibility]
Number of Pareto solutions: 150
Validity range: [0.0058, 0.9890]
Similarity range: [0.0000, 0.7714]
Sparsity range: [0.0000, 2.0000]
Plausibility range: [0.0058, 0.1270]
```