1. Two-dimensional data

In [ ]:
```
import matplotlib.pyplot as plt
from sklearn.datasets import make_moons
from scipy.stats import multivariate_normal
import numpy as np
```

1. Two-dimensional Histogram

$$p(x_i, y_j) = \frac{n_{ij}}{N}$$

$$xp(x_i, y_j) \propto \frac{n_{ij}}{N}$$

In [69]:
```
class Histogram2D:
    def __init__(self, bins=20, range=None):
        self.bins = bins
        self.range = range

    def fit(self, X):
        hist, x_edges, y_edges = np.histogram2d(X[:,0], X[:,1],
                                                bins=self.bins,
                                                range=self.range)

        self.hist = hist / np.sum(hist)
        self.x_edges = x_edges
        self.y_edges = y_edges

        self.hx = x_edges[1] - x_edges[0]
        self.hy = y_edges[1] - y_edges[0]
        return self

    def sample(self, n_samples):
        probs = self.hist.flatten()
        probs /= np.sum(probs)

        idx = np.random.choice(len(probs), size=n_samples, p=probs)
        ix = idx // self.bins
        iy = idx % self.bins

        xs = self.x_edges[ix] + np.random.rand(n_samples) * self.hx
        ys = self.y_edges[iy] + np.random.rand(n_samples) * self.hy

        samples = np.stack([xs, ys], axis=1)
        return samples

    def score_samples(self, X):
        ix = np.searchsorted(self.x_edges, X[:,0], side='right') - 1
        iy = np.searchsorted(self.y_edges, X[:,1], side='right') - 1

        ix = np.clip(ix, 0, self.bins - 1)
        iy = np.clip(iy, 0, self.bins - 1)

        probs = self.hist[ix, iy]
        probs = np.maximum(probs, 1e-12)
        logp = np.log(probs)

        return logp
```

2. Single Gaussian

In [70]:
```
class SingleGaussian:
    def __init__(self):
        self.mean = None
        self.cov = None

    def fit(self, X):
        self.mean = np.mean(X, axis=0)
        diff = X - self.mean
        self.cov = np.cov(diff.T, bias=True)
        return self

    def sample(self, n_samples):
        samples = np.random.multivariate_normal(self.mean, self.cov, size
        return samples

    def score_samples(self, X):
        # log p(x) = -1/2 [ (x-μ)^T Σ^{-1} (x-μ) + log|Σ| + D*log(2π) ]
        D = X.shape[1]
        diff = X - self.mean
        inv_cov = np.linalg.inv(self.cov)
        det_cov = np.linalg.det(self.cov)
        exp_term = np.einsum('ij,jk,ik->i', diff, inv_cov, diff)
        logp = -0.5 * (exp_term + np.log(det_cov) + D * np.log(2 * np.pi)

        return logp
```

3. GMM（Gaussian Mixture Model）

In [115…
```
from scipy.stats import multivariate_normal
class GMM:
    def __init__(self, n_components=3, max_iter=100, tol=1e-4, seed=0):
        self.K = n_components
        self.max_iter = max_iter
        self.tol = tol
        self.seed = seed

    def fit(self, X):
        rng = np.random.default_rng(self.seed)
        N, D = X.shape

        np.random.seed(0)
        self.pi = np.ones(self.K) / self.K
        self.mu = X[np.random.choice(N, self.K, replace=False)]
        self.sigma = np.array([np.cov(X.T) for _ in range(self.K)])

        log_likelihood_old = 0

        for step in range(self.max_iter):
            # E-step
            gamma = np.zeros((N, self.K))
            for k in range(self.K):
                rv = multivariate_normal(mean=self.mu[k],cov=self.sigma[k
                gamma[:, k] = self.pi[k] * rv.pdf(X)
            gamma /= np.sum(gamma, axis=1, keepdims=True)

            # M-step
            Nk = np.sum(gamma, axis=0)
            self.pi = Nk / N
            self.mu = (gamma.T @ X) / Nk[:, np.newaxis]
            self.sigma = np.zeros((self.K, D, D))
            for k in range(self.K):
                diff = X - self.mu[k]
                self.sigma[k] = (gamma[:, k][:, np.newaxis] * diff).T @ d
                self.sigma[k] = 0.5*(self.sigma[k] + self.sigma[k].T)
                self.sigma[k] += 1e-6*np.eye(D)

            log_likelihood = np.sum(np.log(np.sum([
                self.pi[k] * multivariate_normal.pdf(X, self.mu[k], self.
                for k in range(self.K)
            ], axis=0)))
            if abs(log_likelihood - log_likelihood_old) < self.tol:
                break
            log_likelihood_old = log_likelihood
        return self

    def sample(self, n_samples):
        component = np.random.choice(self.K, size=n_samples, p=self.pi)
        samples = np.array([
            np.random.multivariate_normal(self.mu[k], self.sigma[k])
            for k in component
        ])
        return samples

    def score_samples(self, X):
        pdf = np.sum([
            self.pi[k] * multivariate_normal.pdf(X, self.mu[k], self.sigm
            for k in range(self.K)
        ], axis=0)
        return np.log(pdf + 1e-12)
```

4. KDE (Kernel Density Estimation) with a Gaussian Kernel

In [118…

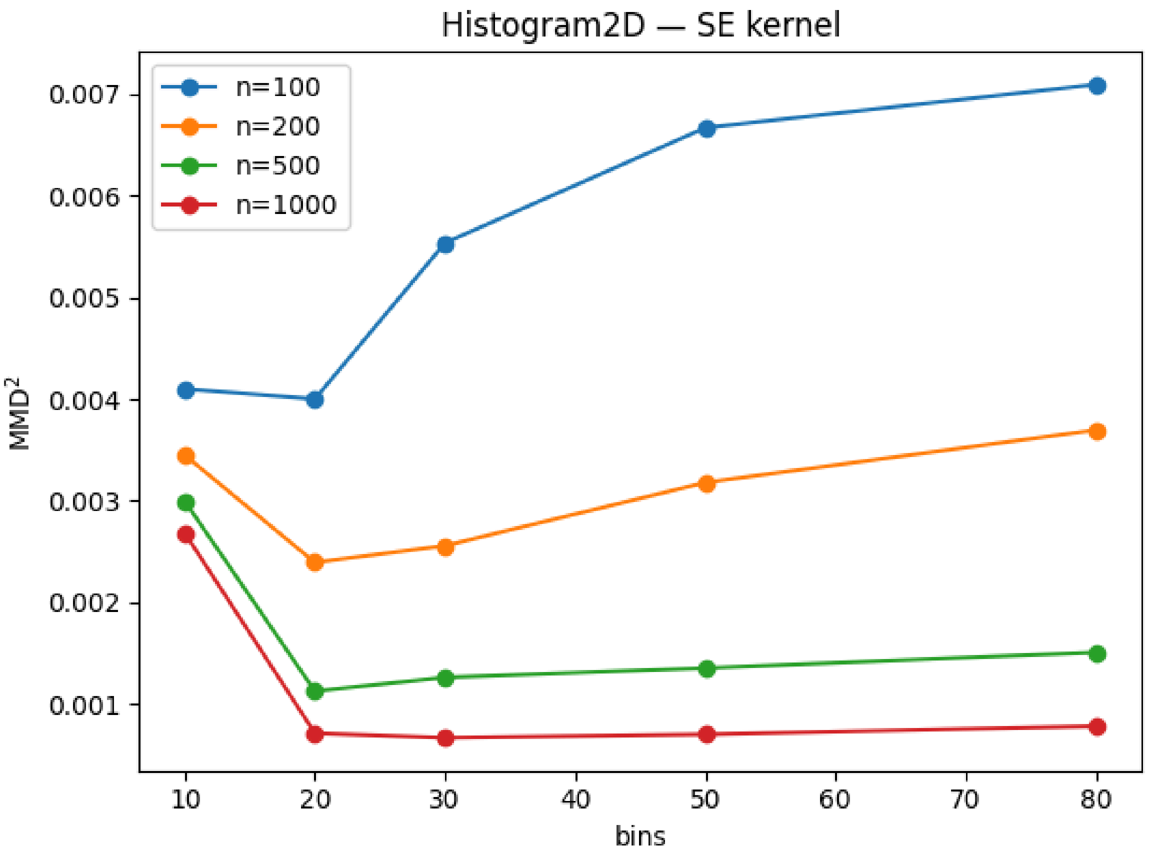
```
class GaussianKDE:
    def __init__(self, bandwidth=0.2):
        self.bandwidth = bandwidth
        self.X_train = None
        self.N = None
        self.D = None

    def fit(self, X):
        self.X_train = X
        self.N, self.D = X.shape
        return self

    def score_samples(self, X):
        h = self.bandwidth
        N, D = self.N, self.D
        Xq = X[:, None, :]
        Xtrain = self.X_train[None, :, :]

        diff = Xq - Xtrain
        dist2 = np.sum(diff**2, axis=2)

        kernel_vals = np.exp(-0.5 * dist2 / (h**2))

        norm_const = (2 * np.pi)**(D/2) * (h**D) * N
        p = np.sum(kernel_vals, axis=1) / norm_const

        return np.log(p + 1e-12)

    def sample(self, n_samples):
        idx = np.random.choice(self.N, size=n_samples, replace=True)
        centers = self.X_train[idx]
        noise = np.random.randn(n_samples, self.D) * self.bandwidth
        return centers + noise
```

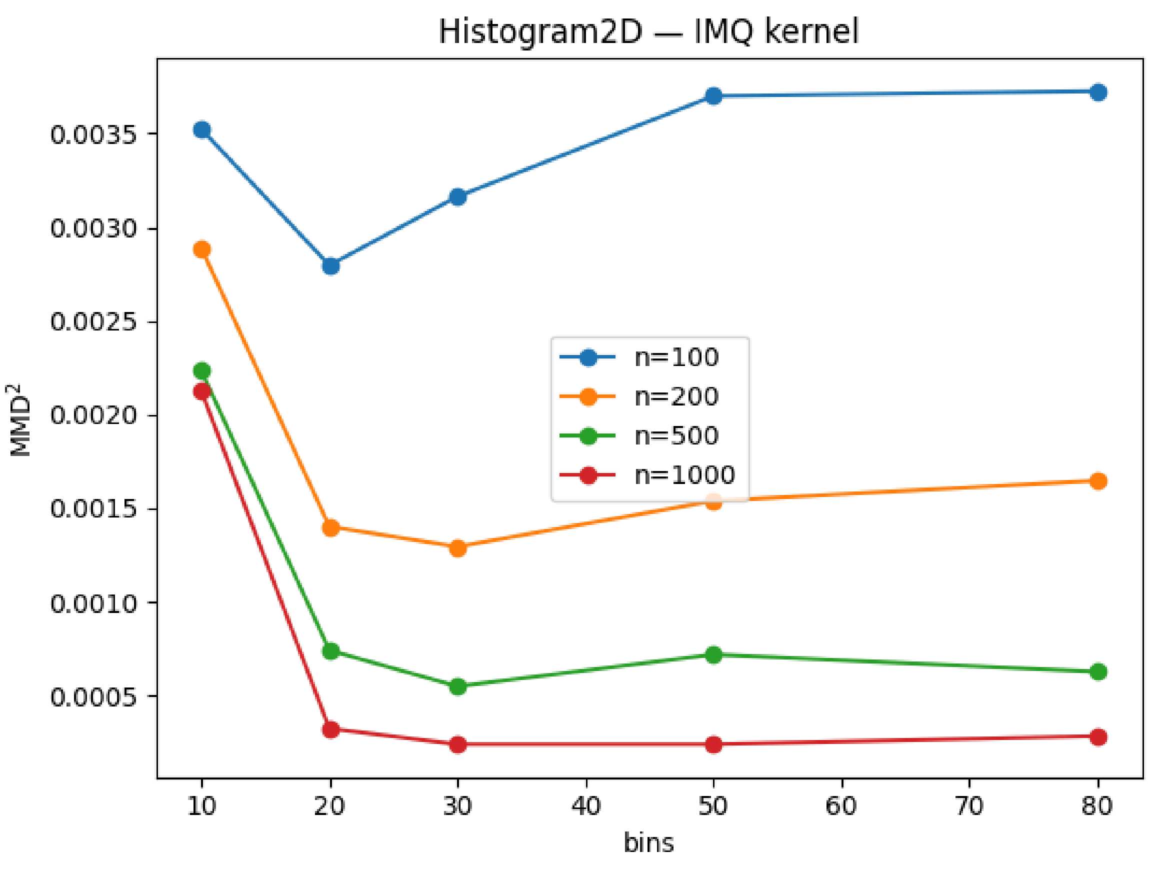
In [ ]:
```
import numpy as np

def _pdist2(X, Y):
    # (n,d),(m,d)->(n,m) 的两两平方欧氏距离
    XX = (X**2).sum(1, keepdims=True)
    YY = (Y**2).sum(1, keepdims=True).T
    d2 = XX + YY - 2 * X @ Y.T
    return np.maximum(d2, 0.0)  # 数值安全

def mmd2_unbiased(X, Y, h=1.0, kernel='se'):
    """无偏 MMD^2，Kxx/Kyy 去掉对角线，分母 n(n-1)/m(m-1)"""
    n, m = len(X), len(Y)
    dxx = _pdist2(X, X)
    dyy = _pdist2(Y, Y)
    dxy = _pdist2(X, Y)

    if kernel == 'se':
        Kxx = np.exp(-dxx/(h*h))
        Kyy = np.exp(-dyy/(h*h))
        Kxy = np.exp(-dxy/(h*h))
    elif kernel == 'imq':
        Kxx = 1.0/np.sqrt(1.0 + dxx/(h*h))
        Kyy = 1.0/np.sqrt(1.0 + dyy/(h*h))
        Kxy = 1.0/np.sqrt(1.0 + dxy/(h*h))
    else:
        raise ValueError("kernel must be 'se' or 'imq'")

    np.fill_diagonal(Kxx, 0.0)
    np.fill_diagonal(Kyy, 0.0)

    term_x = Kxx.sum()/(n*(n-1))
    term_y = Kyy.sum()/(m*(m-1))
    term_xy = 2.0*Kxy.mean()
    return term_x + term_y - term_xy

def median_heuristic(X, max_n=800):
    idx = np.random.choice(len(X), size=min(max_n, len(X)), replace=False
    Z = X[idx]
    d2 = _pdist2(Z, Z)
    med = np.median(d2[np.triu_indices_from(d2, k=1)])
    return np.sqrt(0.5*med)
```

In [110…
```python
def make_data(n, noise=0.1, seed=0):
    X, _ = make_moons(n_samples=n, noise=noise, random_state=seed)
    return X.astype(float)

X_test = make_data(2000, noise=0.1, seed=123)

train_sizes = [100, 200, 500, 1000]
hist_bins_list = [10, 20, 30, 50, 80]
K_list = [1, 2, 3, 5, 8, 12]
kde_bandwidth_list = [0.05, 0.1, 0.2, 0.3]

def plot_curves(results_dict, title):
    """
    results_dict: {label: {"x": list_sizes, "y": list_values}}
    """
    for label, d in results_dict.items():
        plt.plot(d["x"], d["y"], marker="o", label=label)
    plt.xlabel("Train size")
    plt.ylabel("MMD$^2$")
    plt.title(title)
    plt.legend()
    plt.tight_layout()
    plt.show()

def eval_hist_over_bins(train_size, bins_list, kernel="se", R=5, fixed_ra
    Xtr_list = [make_data(train_size, noise=0.1, seed=12345+r) for r in r
    mmds = []
    for b in bins_list:
        vals = []
        for r in range(R):
            X_train = Xtr_list[r]
            model = Histogram2D(bins=b, range=fixed_range).fit(X_train)
            X_gen = model.sample(2000)
            vals.append(mmd2_unbiased(X_test, X_gen, h=h_fixed, kernel=ke
        mmds.append(float(np.mean(vals)))
    return {"x": bins_list, "y": mmds, "label": f"n={train_size}", "kerne


def plot_results_group_bins(group, title_prefix):
    for ker in ("se", "imq"):
        subset = [g for g in group if g["kernel"] == ker]
        results = {g["label"]: {"x": g["x"], "y": g["y"]} for g in subset
        for label, d in results.items():
            plt.plot(d["x"], d["y"], marker="o", label=label)
        plt.xlabel("bins")
        plt.ylabel("MMD$^2$")
        plt.title(f"{title_prefix} — {ker.upper()} kernel")
        plt.legend()
        plt.tight_layout()
        plt.show()
```

In [111…
```python
h_fixed = 0.12
pad = 0.2
fixed_range = [(X_test[:,0].min()-pad, X_test[:,0].max()+pad),
               (X_test[:,1].min()-pad, X_test[:,1].max()+pad)]

all_hist = []
for n in train_sizes:
    all_hist.append(eval_hist_over_bins(n, hist_bins_list, kernel="se",
                                            fixed_range=fixed_range, h_fixed=
    all_hist.append(eval_hist_over_bins(n, hist_bins_list, kernel="imq",
                                            fixed_range=fixed_range, h_fixed=
plot_results_group_bins(all_hist, "Histogram2D")
```

```
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: divide by zero encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: overflow encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: invalid value encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
```





Histogram2D — SE kernel

For all training sizes, MMD² drops markedly when we move from 10 to 20 bins and then increases again as the grid gets finer (30–80). Larger training sets consistently achieve lower MMD² across the entire range.

The initial improvement (10 → 20 bins) reflects reduced bias: a very coarse grid cannot capture the curved “two-moons” structure. Beyond 20 bins, variance dominates: many bins become sparsely populated or empty, so the histogram sample generator picks bins that do not represent the test distribution well, which pushes MMD² up. With more data, the variance penalty is smaller, hence the shallower increase.

Histogram2D — IMQ kernel

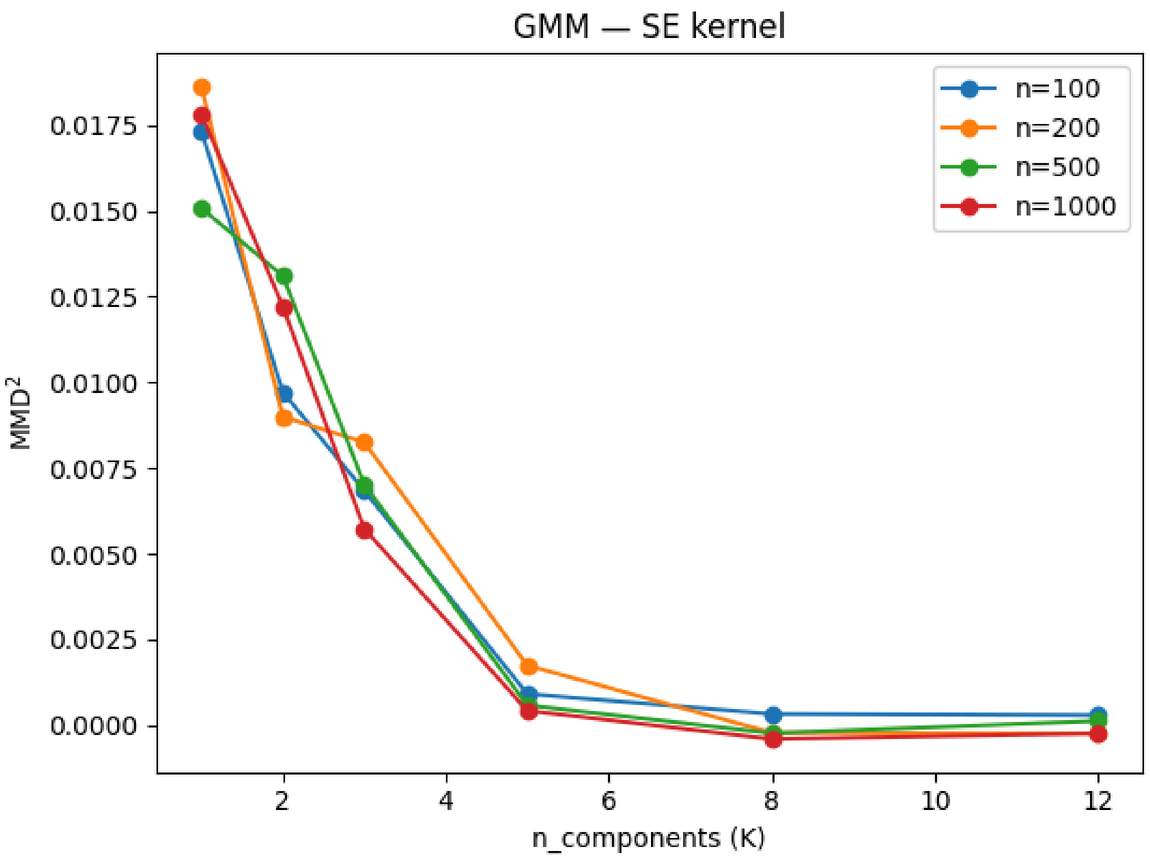
The overall pattern matches the SE plot: a clear drop between 10 and 20 bins, followed by a mild increase as the grid is refined. Absolute MMD² values are smaller than with SE.

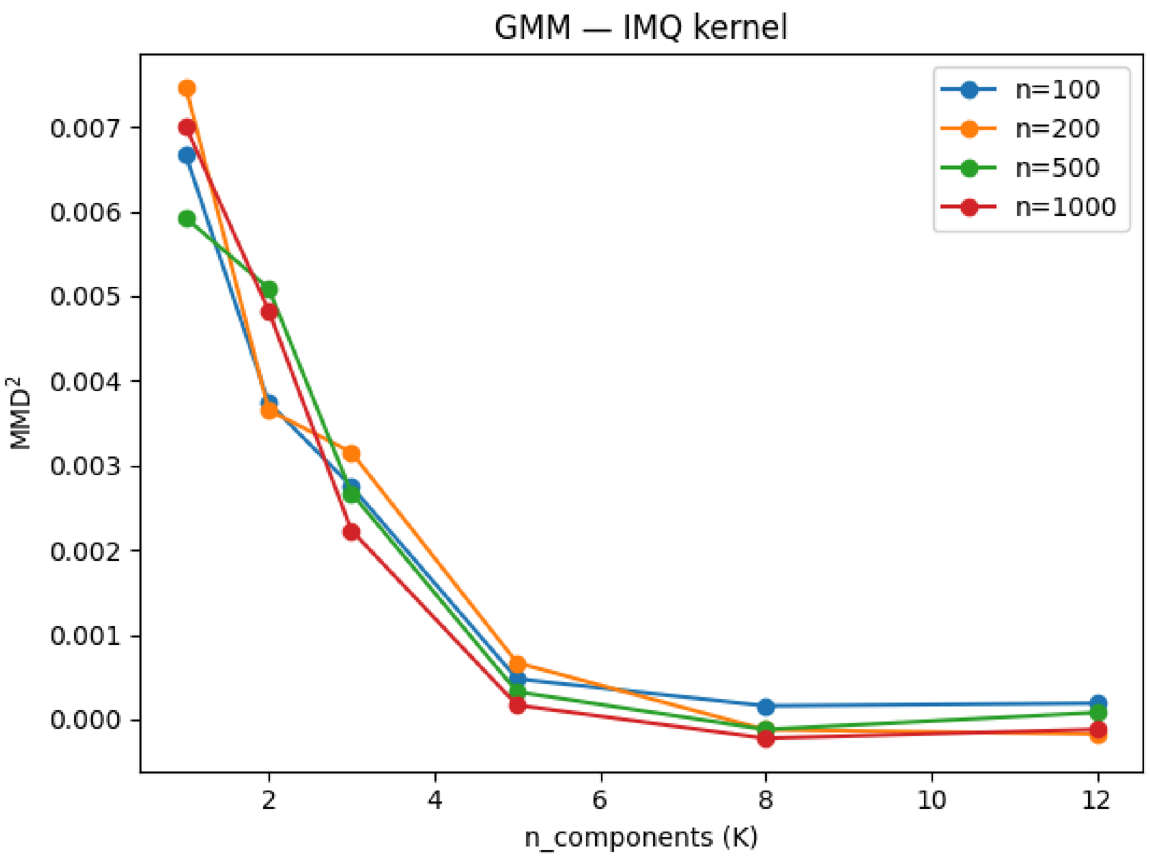
The IMQ kernel weights larger pairwise distances more heavily and is less sensitive to very local misalignments than SE. Consequently, the variance introduced by many tiny bins hurts slightly less in IMQ, hence the lower scale.

In [116…

```
def eval_gmm_over_components(train_size, k_list, kernel="se",
                             R=5, h_fixed=None, seed_base=24680, ngen=200

    # 准备 R 份训练集，且与 K 无关
    Xtr_list = [make_data(train_size, noise=0.1, seed=seed_base + r) for

    mmds = []
    for K in k_list:
        vals = []
        for r in range(R):
            X_train = Xtr_list[r]
            model = GMM(n_components=K, seed=0).fit(X_train)
            X_gen = model.sample(ngen)
            h = h_fixed if h_fixed is not None else median_heuristic(np.v
            vals.append(mmd2_unbiased(X_test, X_gen, h=h, kernel=kernel))
        mmds.append(float(np.mean(vals)))
    return {"x": k_list, "y": mmds, "label": f"n={train_size}", "kernel":

def plot_results_group_components(group, title_prefix):
    for ker in ("se", "imq"):
        subset = [g for g in group if g["kernel"] == ker]
        results = {g["label"]: {"x": g["x"], "y": g["y"]} for g in subset
        for label, d in results.items():
            plt.plot(d["x"], d["y"], marker="o", label=label)
        plt.xlabel("n_components (K)")
        plt.ylabel("MMD$^2$")
        plt.title(f"{title_prefix} — {ker.upper()} kernel")
        plt.legend()
        plt.tight_layout()
        plt.show()


h_fixed = median_heuristic(X_test)  # 固定带宽让横向更可比

all_gmm = []
for n in train_sizes:  # 每条曲线一个训练规模
    all_gmm.append(eval_gmm_over_components(n, K_list, kernel="se",  R=5,
    all_gmm.append(eval_gmm_over_components(n, K_list, kernel="imq", R=5,

plot_results_group_components(all_gmm, "GMM")
```

```
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: divide by zero encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: overflow encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: invalid value encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/400519419
9.py:31: RuntimeWarning: divide by zero encountered in matmul
  self.mu = (gamma.T @ X) / Nk[:, np.newaxis]
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/400519419
9.py:31: RuntimeWarning: overflow encountered in matmul
  self.mu = (gamma.T @ X) / Nk[:, np.newaxis]
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/400519419
9.py:31: RuntimeWarning: invalid value encountered in matmul
  self.mu = (gamma.T @ X) / Nk[:, np.newaxis]
```





GMM — SE kernel

MMD² decreases steeply as the number of components grows from 1 to 5, then flattens around zero (and even dips slightly below zero) for K ≥ 6–12. Larger training sets yield slightly better optima.

A single Gaussian cannot model the two-moon geometry. Increasing K reduces bias by allowing a multi-modal approximation; after 5 components the mixture is flexible enough to closely match the target, and additional components bring diminishing returns. Tiny negative values are again consistent with an unbiased MMD$^2$ estimate around the optimum.

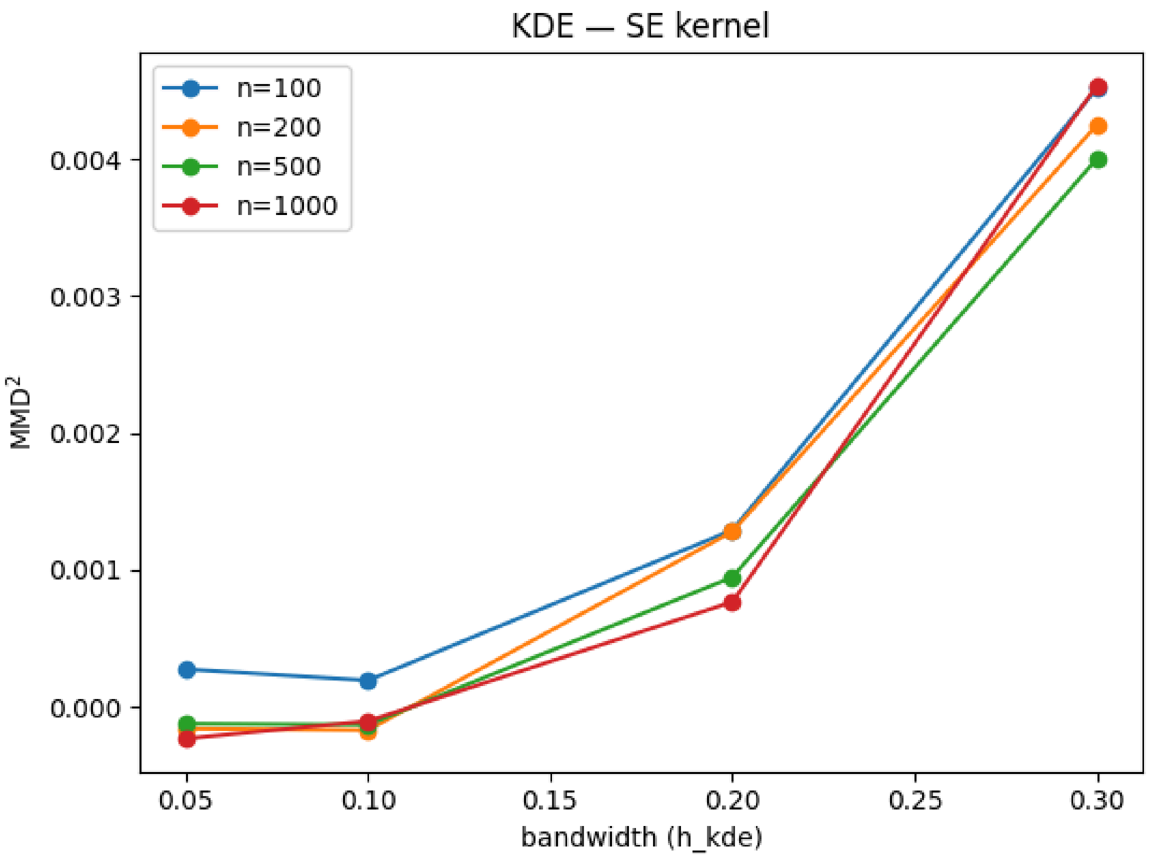
GMM — IMQ kernel

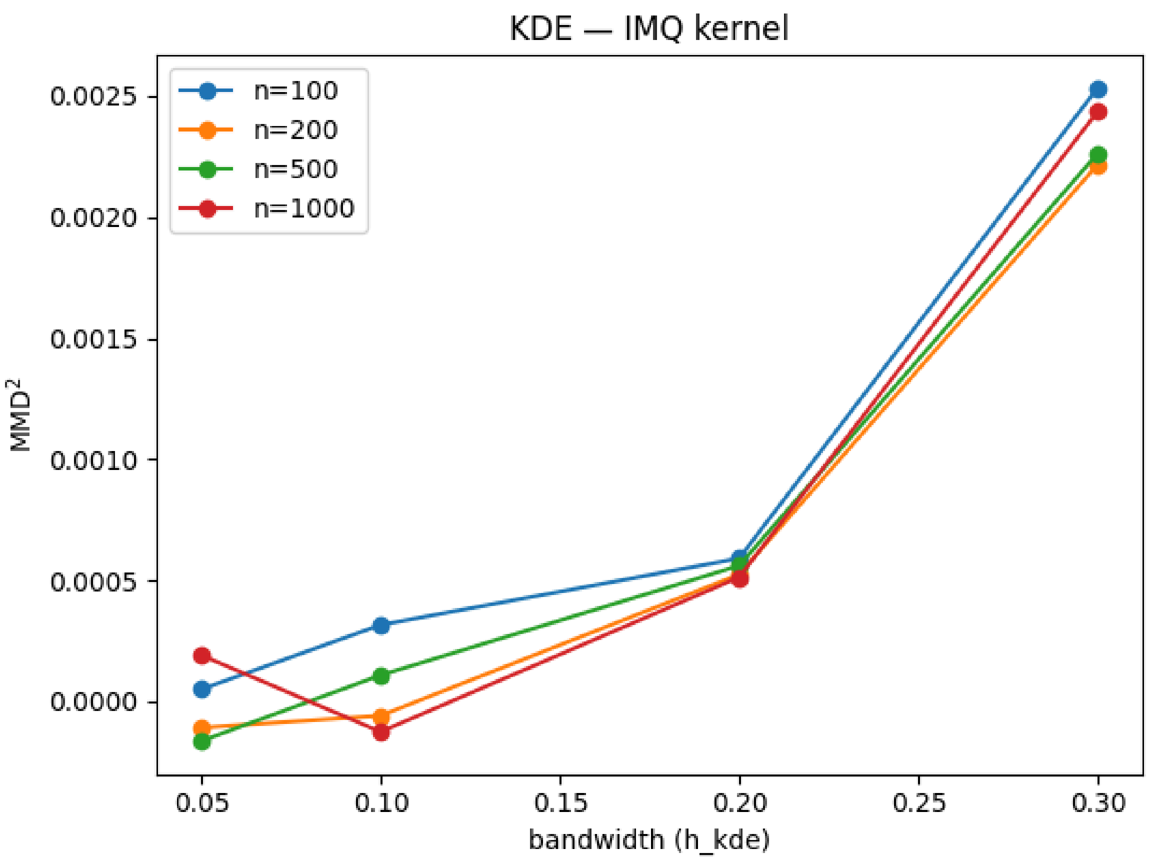
Same qualitative behavior as with SE, at a smaller numerical scale. The optimum is reached around K≈6–8, after which the curve is essentially flat.

IMQ's heavier tail makes it slightly more tolerant to local overfitting; hence the very low (sometimes negative) MMD$^2$ once K is sufficient.

In [ ]:
```python
def eval_kde_over_bandwidth(train_size, bw_list, kernel="se",
                            R=5, seed_base=31415, ngen=2000,
                            h_mmd_fixed=None):
    """
    返回一条曲线：固定 train_size，横轴是 KDE 带宽 (h_kde)。
    - R: 重复次数，降低方差；X_train 对同一 r 在不同 h_kde 下复用
    - h_mmd_fixed: 若提供，则评估 MMD 的带宽固定；否则用合并样本的 median heuris
    """
    # 准备 R 份训练集
    Xtr_list = [make_data(train_size, noise=0.1, seed=seed_base + r) for

    mmds = []
    for h_kde in bw_list:
        vals = []
        for r in range(R):
            X_train = Xtr_list[r]
            model = GaussianKDE(bandwidth=h_kde).fit(X_train)
            X_gen = model.sample(ngen)
            h_mmd = h_mmd_fixed if h_mmd_fixed is not None else median_he
            vals.append(mmd2_unbiased(X_test, X_gen, h=h_mmd, kernel=kern
        mmds.append(float(np.mean(vals)))
    return {"x": bw_list, "y": mmds, "label": f"n={train_size}", "kernel"

def plot_results_group_bandwidth(group, title_prefix):
    for ker in ("se", "imq"):
        subset = [g for g in group if g["kernel"] == ker]
        results = {g["label"]: {"x": g["x"], "y": g["y"]} for g in subset
        for label, d in results.items():
            plt.plot(d["x"], d["y"], marker="o", label=label)
        plt.xlabel("bandwidth (h_kde)")
        plt.ylabel("MMD$^2$")
        plt.title(f"{title_prefix} — {ker.upper()} kernel")
        plt.legend()
        plt.tight_layout()
        plt.show()


bw_list = kde_bandwidth_list
h_mmd_fixed = median_heuristic(X_test)          # 固定 MMD 的带宽，提升横向

all_kde = []
for n in train_sizes:
    all_kde.append(eval_kde_over_bandwidth(n, bw_list, kernel="se",  R=5,
    all_kde.append(eval_kde_over_bandwidth(n, bw_list, kernel="imq", R=5,

plot_results_group_bandwidth(all_kde, "KDE")
```

```
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: divide by zero encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: overflow encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: invalid value encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
```





KDE — SE kernel

MMD² increases monotonically with the bandwidth h (0.05 → 0.30). The best region is at the smallest bandwidths; larger n helps but does not invert the trend.

The moons distribution has thin, curved structures. Small bandwidths capture these manifolds; large bandwidths oversmooth and fill the gap between the moons, producing samples that deviate from the test set, hence larger MMD². With more data, even small h remains stable (variance drops), so the curves for larger n stay low near h=0.05–0.10.

KDE — IMQ kernel

The same monotone increase with bandwidth appears, with slightly smaller magnitudes than SE. For n=1000 and small h the estimates hover around zero and can be marginally negative.

Identical to the SE case: oversmoothing harms alignment with the moon geometry; IMQ's wider sensitivity range lowers the overall scale and masks some local discrepancies.

In [ ]:
```
def sanity_check_sg_vs_gmm1(train_sizes, h_fixed=None, R=5, ngen=2000, ke
    if h_fixed is None:
        h_fixed = median_heuristic(X_test)
    diffs = []
    for n in train_sizes:
        vals = []
        for r in range(R):
            X_train = make_data(n, noise=0.1, seed=10_000*n + r)
            sg  = SingleGaussian().fit(X_train)
            g1  = GMM(n_components=1).fit(X_train)
            XgA = sg.sample(ngen);  mmdA = mmd2_unbiased(X_test, XgA, h=h
            XgB = g1.sample(ngen);  mmdB = mmd2_unbiased(X_test, XgB, h=h
            vals.append(abs(mmdA - mmdB))
        diffs.append((n, float(np.mean(vals))))
    return diffs

print(sanity_check_sg_vs_gmm1(train_sizes, kernel="se"))
print(sanity_check_sg_vs_gmm1(train_sizes, kernel="imq"))
```

```
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: divide by zero encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
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1.py:7: RuntimeWarning: overflow encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: invalid value encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
[(100, 0.0006641205423078666), (200, 0.001032239609767438), (500, 0.001320
968018227231), (1000, 0.0003107865357393491)]
[(100, 0.00027353478721581226), (200, 0.00038382705668977836), (500, 0.000
23641252889725629), (1000, 0.00021200474914424562)]
```
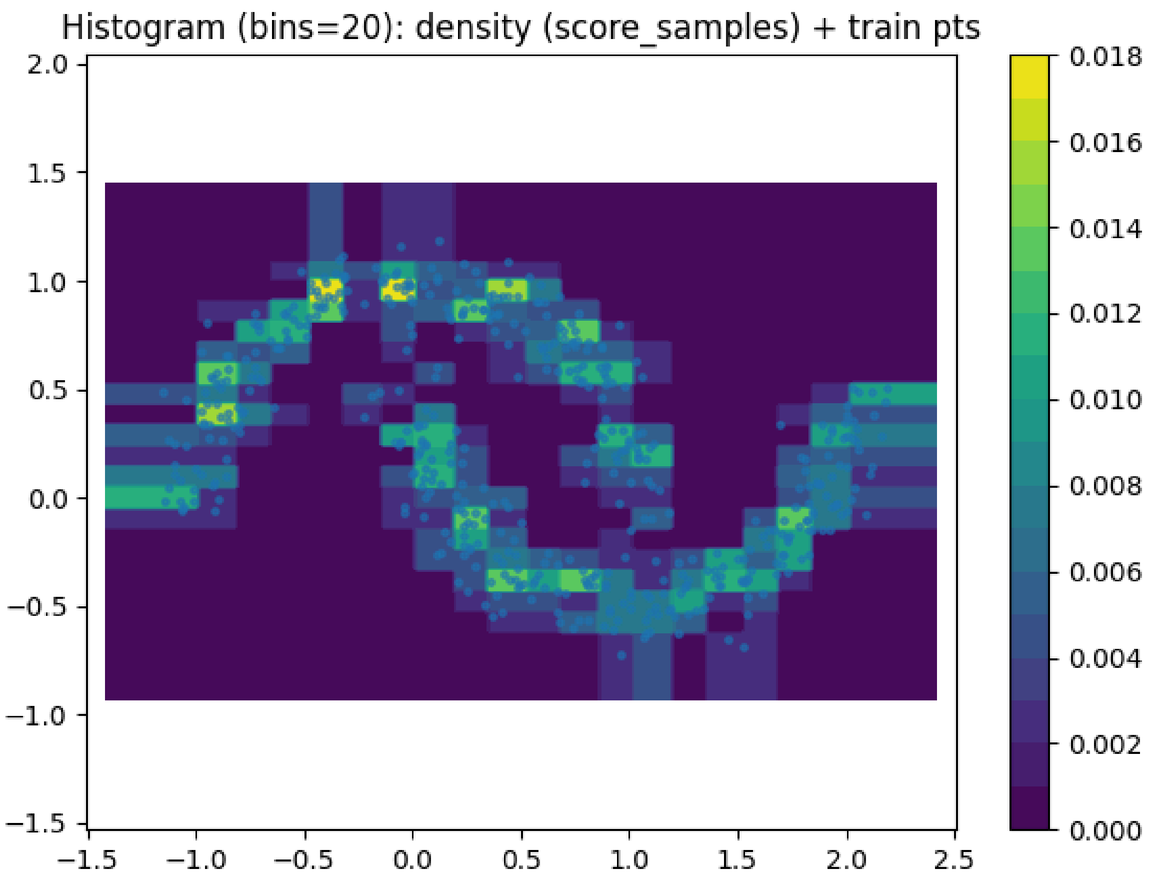
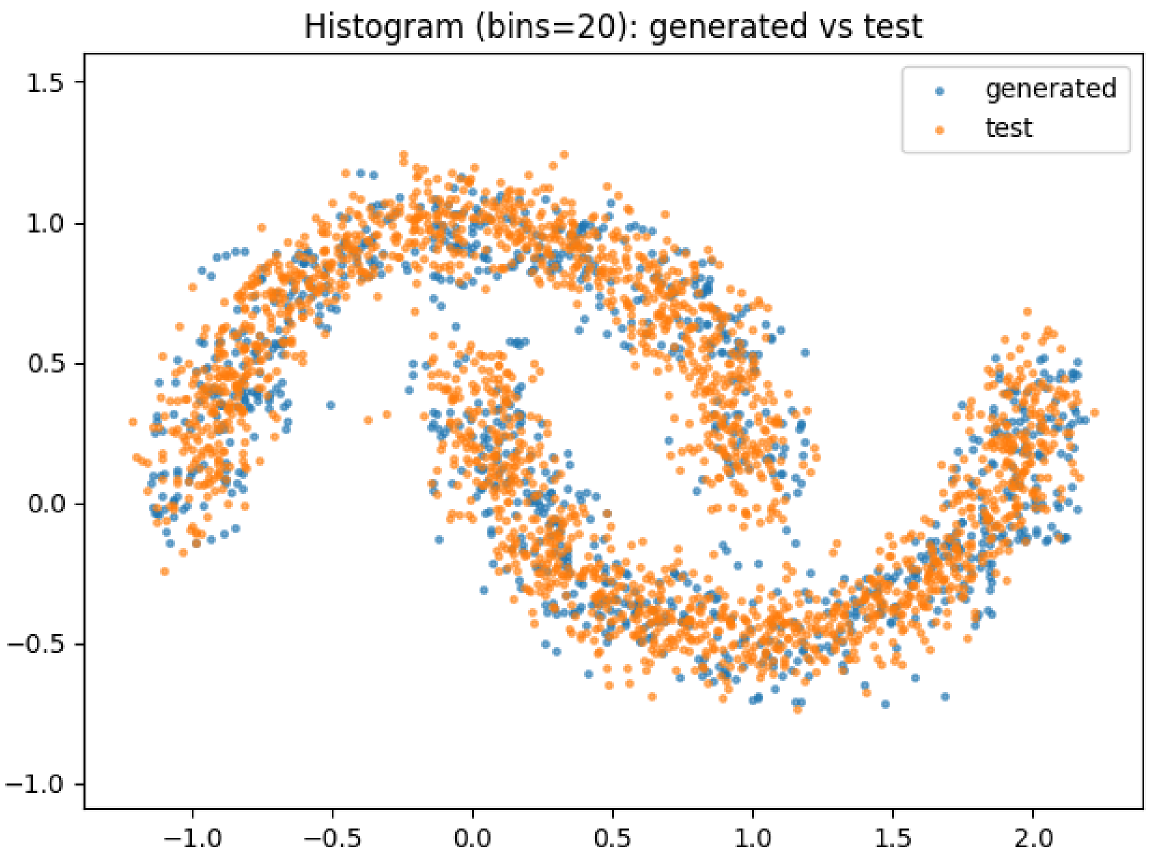
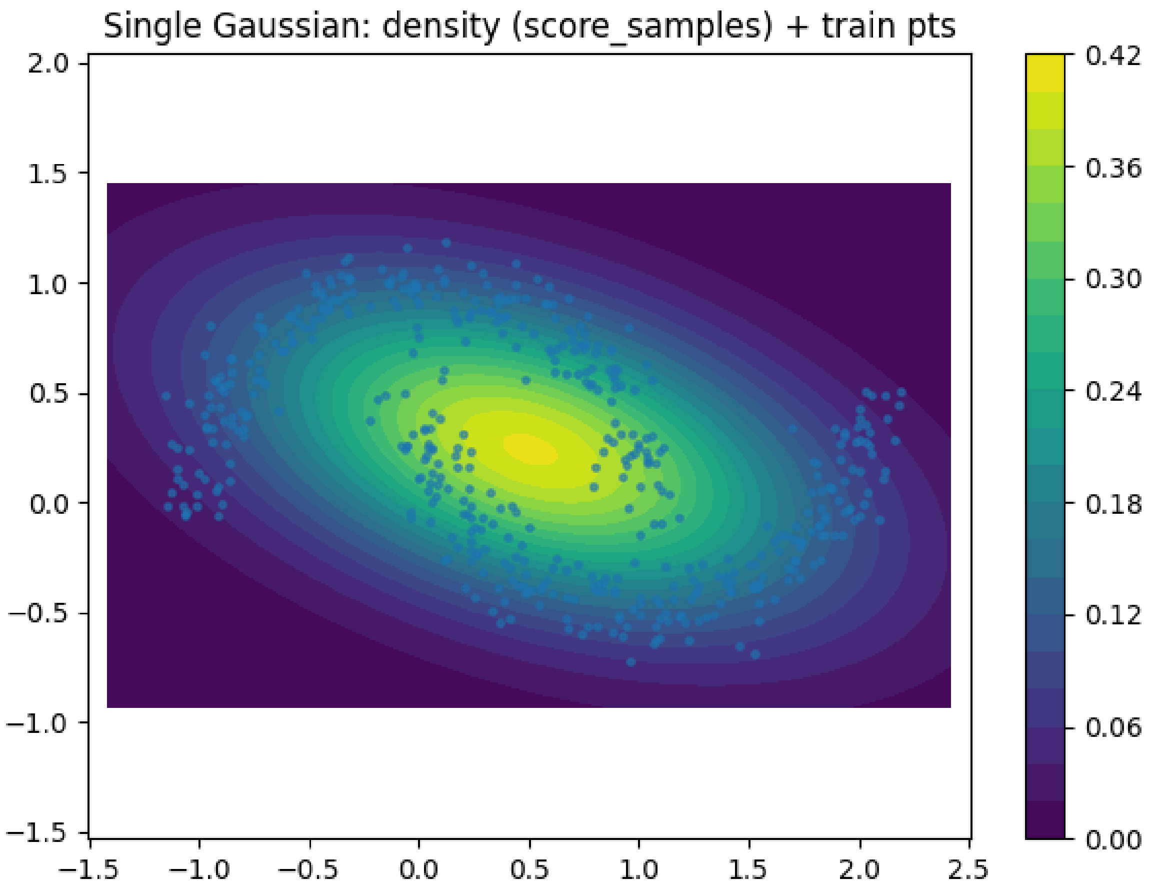
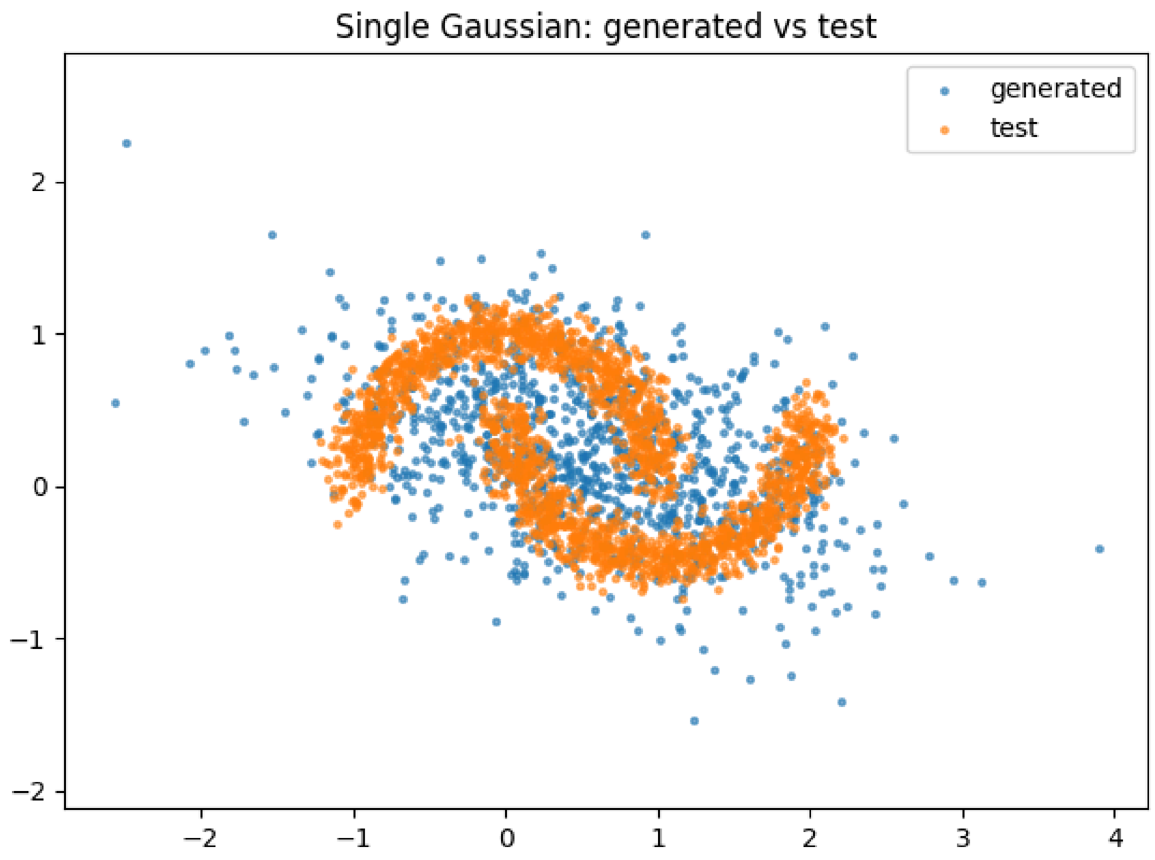

In [ ]:
```
def make_grid(X, n=150, pad=0.2):
    lo = X.min(axis=0) - pad
    hi = X.max(axis=0) + pad
    xs = np.linspace(lo[0], hi[0], n)
    ys = np.linspace(lo[1], hi[1], n)
    GX, GY = np.meshgrid(xs, ys)
    G = np.column_stack([GX.ravel(), GY.ravel()])
    return xs, ys, GX, GY, G

def visualize_model(model, X_train, n_gen=1000, title="Model"):
    xs, ys, GX, GY, G = make_grid(np.vstack([X_train, X_test]))
    Z = np.exp(model.score_samples(G)).reshape(GX.shape)

    # (i) 密度等高线
    plt.contourf(GX, GY, Z, levels=20)
    plt.colorbar()
    plt.scatter(X_train[:, 0], X_train[:, 1], s=6, alpha=0.6)
    plt.axis("equal")
    plt.title(f"{title}: density (score_samples) + train pts")
    plt.tight_layout()
    plt.show()

    # (ii) 生成样本散点
    X_gen = model.sample(n_gen)
    plt.scatter(X_gen[:, 0], X_gen[:, 1], s=6, alpha=0.6, label="generate
    plt.scatter(X_test[:, 0], X_test[:, 1], s=6, alpha=0.6, label="test")
    plt.axis("equal")
    plt.legend()
    plt.title(f"{title}: generated vs test")
    plt.tight_layout()
    plt.show()


X_tr = make_data(500, noise=0.1, seed=7)
```

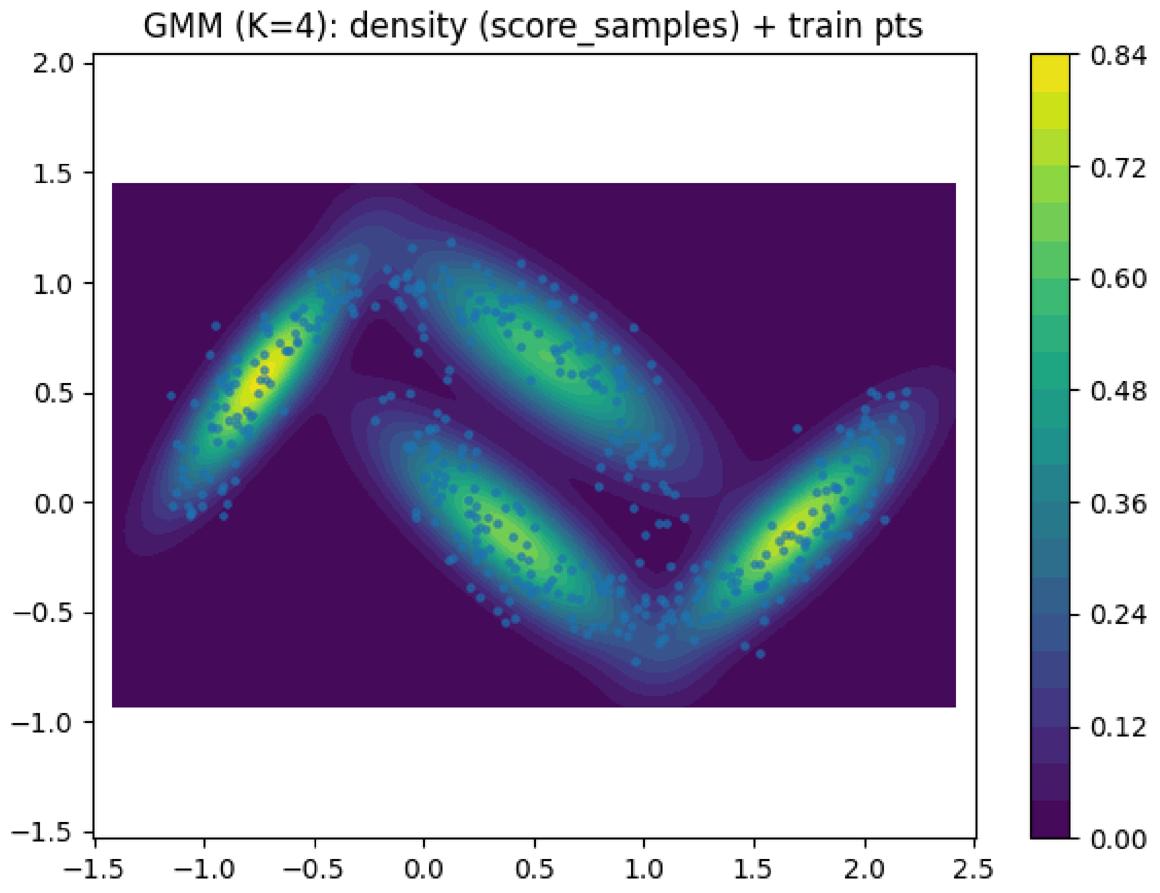
```
models_show = [
    ("Histogram (bins=20)", Histogram2D(bins=20).fit(X_tr)),
    ("Single Gaussian",     SingleGaussian().fit(X_tr)),
    ("GMM (K=4)",           GMM(n_components=4, seed=0).fit(X_tr)),
    ("KDE (h=0.15)",         GaussianKDE(bandwidth=0.15).fit(X_tr)),
]

for name, mdl in models_show:
    visualize_model(mdl, X_tr, title=name)
```

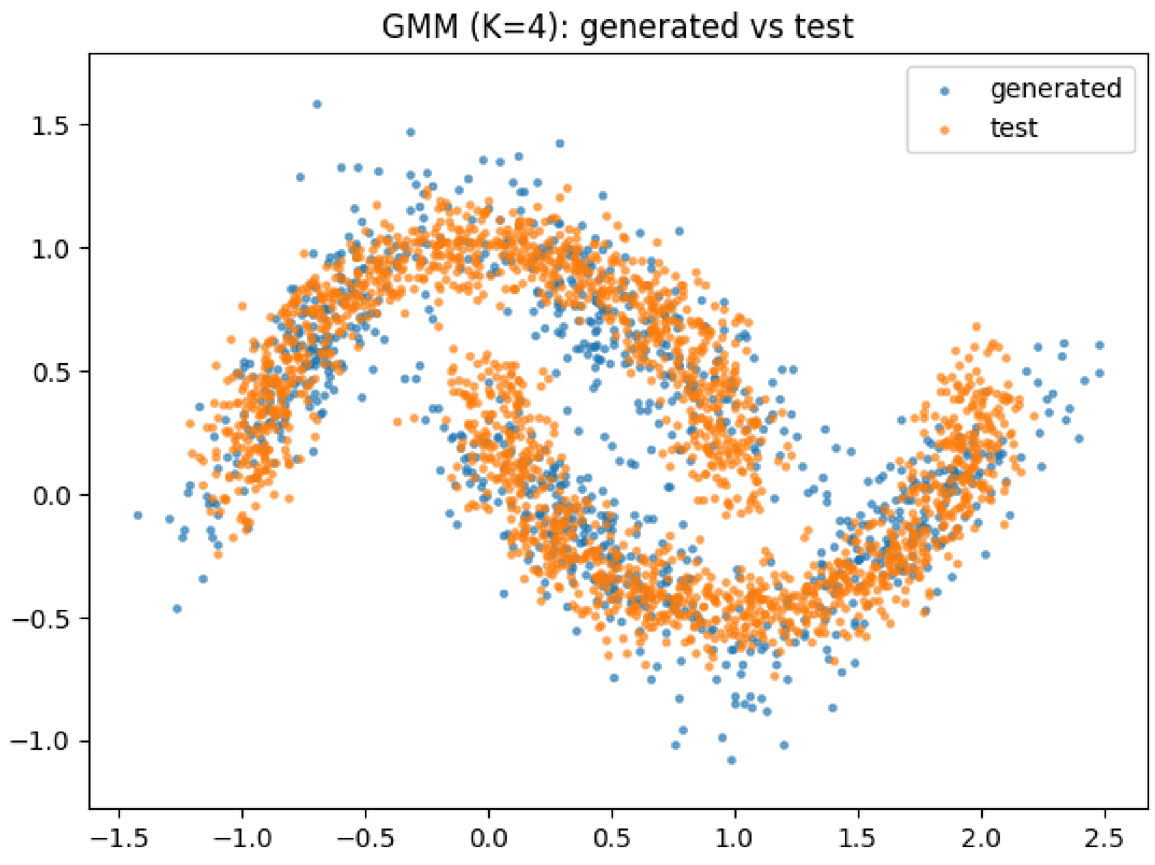


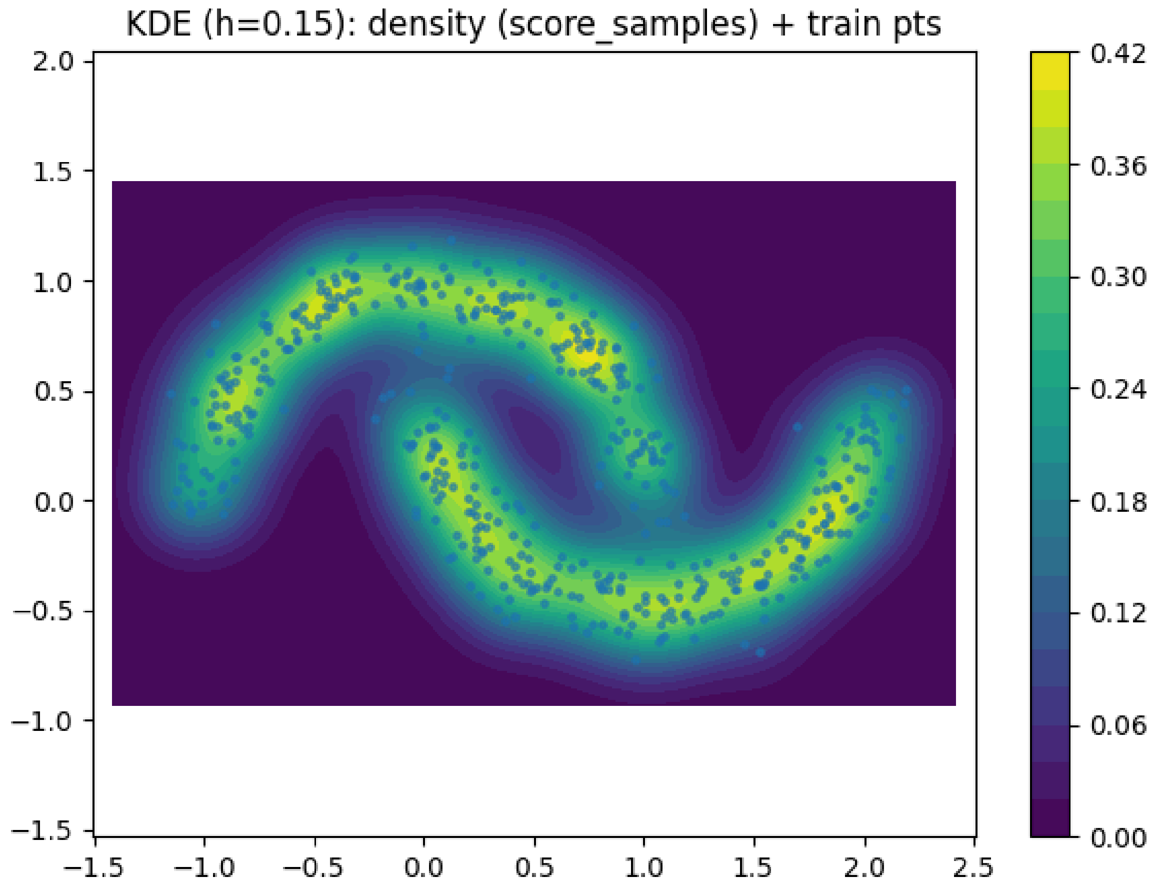

Histogram (bins=20): generated vs test
generated
test
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

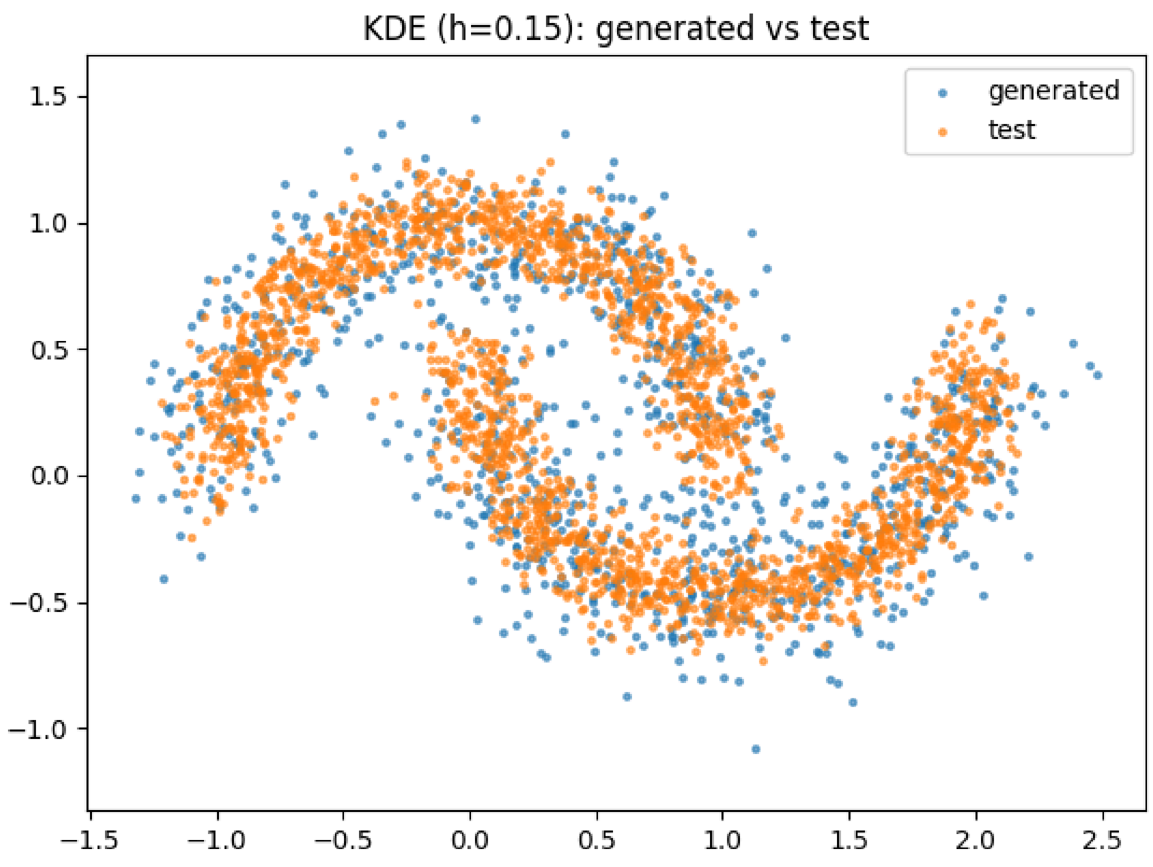

Single Gaussian: density (score_samples) + train pts
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00


Single Gaussian: generated vs test
generated
test
2
1
0
−1
−2
−2
−1
0
1
2
3
4


GMM (K=4): density (score_samples) + train pts
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
0.84
0.72
0.60
0.48
0.36
0.24
0.12
0.00


GMM (K=4): generated vs test
generated
test
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5


KDE (h=0.15): density (score_samples) + train pts
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00



Histogram (bins=20): density (score_samples) + train points

The piecewise-constant nature of the 2D histogram is visible: density blocks align with grid cells and create jagged boundaries. Still, the model captures the two arcs fairly well at this resolution.

Histogram (bins = 20): generated vs test

Generated samples broadly follow the moons and match the global shape.Small clumps near bin edges and a few tiny gaps reflect uniform sampling inside selected bins.

Single Gaussian: density (score_samples) + train points

Contours are elliptical and fill the central gap, which contradicts the bimodal curved structure of the moons. This shows strong model bias: a single Gaussian cannot represent the non-elliptical, multi-modal geometry.

Single Gaussian: generated vs test

Samples concentrate in the middle and spill between the two arcs, clearly misaligning with the test set. This is a bad model and explains the large MMD² obtained for K=1 vs the moons.

GMM (K = 4): density (score_samples) + train points

Multiple elongated components start to trace the arcs and carve out the low-density gap. Some leakage remains between the moons and at the tips, but the global pattern is largely correct. Increasing K typically tightens the fit.

GMM (K = 4): generated vs test

Generated points align closely with the test set. In the MMD² curves the optimum appears around K≈6–8, where these residual errors further diminish.

KDE (h = 0.15): density (score_samples) + train points

Gaussian KDE produces a smooth density that follows the curved manifolds and maintains the central gap. With this bandwidth the bias–variance trade-off is favorable.

KDE (h = 0.15): generated vs test

Generated samples are almost indistinguishable from the test points. Among the four models, KDE with a small h gives the best visual match.

2. Higher-dimensional data

In [157…

```
from sklearn.datasets import load_digits
from sklearn.mixture import GaussianMixture
from sklearn.neighbors import KernelDensity
from sklearn.ensemble import RandomForestClassifier
from joblib import Parallel, delayed
```

In [158…

```
rng = np.random.RandomState(42)
digits = load_digits()
X_train, y_train = digits.data, digits.target
n_features = X_train.shape[1]
test_size = 2000

gmm_components = [1, 2, 3, 4, 5, 7, 10, 15, 20, 30, 50, 100]
kde_bandwidths = [0.001, 0.002, 0.005, 0.0075, 0.01, 0.02, 0.05, 0.075, 0
n_mins = [5, 10, 20, 50, 100, 200]

# Containers to store MMD results
mmd_results = {
    'GMM': {'parameters': [] , 'mmd_se': [], 'mmd_imq': [], 'model': []},
    'KDE': {'parameters': [], 'mmd_se': [], 'mmd_imq': [], 'model': []},
    'DF' : {'parameters': [], 'mmd_se': [], 'mmd_imq': [], 'model': []}
}

# 密度森林 (density forest)
class Node: ...

class DensityTree:
    def __init__(self, n_min=10):
        self.n_min = n_min
        self.kernal = {'count': [], 'mean': [], 'cov': []}
```

```python
    def fit(self, features, D_try=None):
        N, D = features.shape
        if D_try is None:
            D_try = int(np.sqrt(D))  # 每次split随机考虑的特征数

        self.root = Node(); self.root.features = features
        stack = [self.root]
        while stack:
            node = stack.pop()
            active_indices = self.select_active_indices(D, D_try)
            left, right = self.make_split_node(node, active_indices)
            if left is None:  # no split found
                self.make_leaf_node(node)
            else:
                stack.extend([left, right])

        # 组装为高斯混合的权重/均值/协方差，便于采样
        self.weights_ = np.array(self.kernal['count'], dtype=float)
        self.weights_ = self.weights_ / self.weights_.sum()
        self.means_ = np.array(self.kernal['mean'])
        self.covariances_ = np.array(self.kernal['cov'])
        self.n_components = self.weights_.shape[0]

    def make_split_node(self, node, indices):
        l_min = float('inf'); j_min = None; t_min = None
        for j in indices:
            thresholds = self.find_thresholds(node, j)
            for t in thresholds:
                loss = self.compute_loss_for_split(node, j, t)
                if loss < l_min:
                    l_min, j_min, t_min = loss, j, t
        if j_min is None:
            return None, None
        left, right = self.make_children(node, j_min, t_min)
        node.left, node.right = left, right
        node.split_index, node.threshold = j_min, t_min
        return left, right

    def select_active_indices(self, D, D_try):
        return rng.choice(np.arange(D), size=D_try, replace=False)

    def find_thresholds(self, node, j):
        # 叶子最少数量约束，保证两边至少 n_min
        if node.features.shape[0] < 2*self.n_min:
            return []
        sort = np.sort(node.features[:, j])
        t = (sort[:-1] + sort[1:]) / 2
        if self.n_min > 1:
            t = t[(self.n_min-1): (-self.n_min+1)]
        return t

    def make_children(self, node, j, t):
        left = Node(); right = Node()
        left.features  = node.features[node.features[:, j] <= t]
        right.features = node.features[node.features[:, j] >  t]
        return left, right

    def entropy_gaussian(self, features):
        # 加微扰，防 det(cov) = 0
        cov = np.cov(features.T)
        cov = cov + 1e-6*np.eye(cov.shape[0])
        sign, logdet = np.linalg.slogdet(cov)
        if sign <= 0:  # 极端退化
            return float('inf')
        # H(N(μ,Σ)) = 0.5 * log((2πe)^d detΣ)
        d = features.shape[1]
        return 0.5 * (d*np.log(2*np.pi*np.e) + logdet)

    def compute_loss_for_split(self, node, j, t):
        l_resp = node.features[node.features[:, j] <= t]
        r_resp = node.features[node.features[:, j] >  t]
        if (l_resp.shape[0] < self.n_min) or (r_resp.shape[0] < self.n_mi
            return float('inf')
        return self.entropy_gaussian(l_resp) + self.entropy_gaussian(r_re

    def make_leaf_node(self, node):
        self.kernal['count'].append(node.features.shape[0])
        self.kernal['mean'].append(node.features.mean(0))
        cov = np.cov(node.features.T) + 1e-6*np.eye(node.features.shape[1
        self.kernal['cov'].append(cov)

    def sample(self, n_samples):
        idx = rng.choice(self.n_components, size=n_samples, p=self.weight
        chunks = []
        for k in range(self.n_components):
            n_k = np.sum(idx == k)
            if n_k:
                chunks.append(rng.multivariate_normal(self.means_[k], sel
        samples = np.vstack(chunks)
        rng.shuffle(samples)
        return samples

def bootstrap_sampling(features):
    N = features.shape[0]
    inds = rng.choice(N, N, replace=True)
    return features[inds]
```

In [159…

```
class DensityForest:
    def __init__(self, n_trees=10, n_min=10):
        self.n_trees = n_trees
        self.trees = [DensityTree(n_min) for _ in range(n_trees)]

    def fit(self, features):
        self.trees = Parallel(n_jobs=-1)(
            delayed(self._fit_tree)(tree, features) for tree in self.tree
        )

    def _fit_tree(self, tree, features):
        tree.fit(bootstrap_sampling(features))
        return tree

    def sample(self, n_samples):
        # 先按树均匀抽，再在每棵树内用其叶GMM采样
        idx = rng.choice(self.n_trees, size=n_samples)
        chunks = []
        for t, tree in enumerate(self.trees):
            n_k = np.sum(idx == t)
            if n_k:
                chunks.append(tree.sample(n_k))
        samples = np.vstack(chunks)
        rng.shuffle(samples)
        return samples
```

In [160…

```
# 训练 & MMD² 评估

for n_comp in gmm_components:
    gmm = GaussianMixture(n_components=n_comp, init_params='k-means++', r
    gmm.fit(X_train)
    samples, _ = gmm.sample(test_size)
    mmd_se  = mmd2_unbiased(samples, X_train, h=1.0, kernel='se')
    mmd_imq = mmd2_unbiased(samples, X_train, h=1.0, kernel='imq')
    mmd_results['GMM']['parameters'].append(n_comp)
    mmd_results['GMM']['mmd_se'].append(float(mmd_se))
    mmd_results['GMM']['mmd_imq'].append(float(mmd_imq))
    mmd_results['GMM']['model'].append(gmm)

for bw in kde_bandwidths:
    kde = KernelDensity(kernel='gaussian', bandwidth=bw)
    kde.fit(X_train)
    samples = kde.sample(test_size, random_state=42)
    mmd_se  = mmd2_unbiased(samples, X_train, h=1.0, kernel='se')
    mmd_imq = mmd2_unbiased(samples, X_train, h=1.0, kernel='imq')
    mmd_results['KDE']['parameters'].append(bw)
    mmd_results['KDE']['mmd_se'].append(float(mmd_se))
    mmd_results['KDE']['mmd_imq'].append(float(mmd_imq))
    mmd_results['KDE']['model'].append(kde)

for n_min in n_mins:
    df = DensityForest(n_trees=10, n_min=n_min)
    df.fit(X_train)
    samples = df.sample(test_size)
    mmd_se  = mmd2_unbiased(samples, X_train, h=1.0, kernel='se')
    mmd_imq = mmd2_unbiased(samples, X_train, h=1.0, kernel='imq')
    mmd_results['DF']['parameters'].append(n_min)
    mmd_results['DF']['mmd_se'].append(float(mmd_se))
    mmd_results['DF']['mmd_imq'].append(float(mmd_imq))
    mmd_results['DF']['model'].append(df)
```

```
/Users/xinyi/Desktop/node2/node2/lib/python3.13/site-packages/sklearn/util
s/extmath.py:203: RuntimeWarning: divide by zero encountered in matmul
  ret = a @ b
/Users/xinyi/Desktop/node2/node2/lib/python3.13/site-packages/sklearn/util
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  current_pot = closest_dist_sq @ sample_weight
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/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
1.py:7: RuntimeWarning: divide by zero encountered in matmul
  d2 = XX + YY - 2 * X @ Y.T
/var/folders/jq/_3nxnjcd16nb8qvqvyf92n7r0000gn/T/ipykernel_97944/369752590
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  sign, logdet = _umath_linalg.slogdet(a, signature=signature)
```
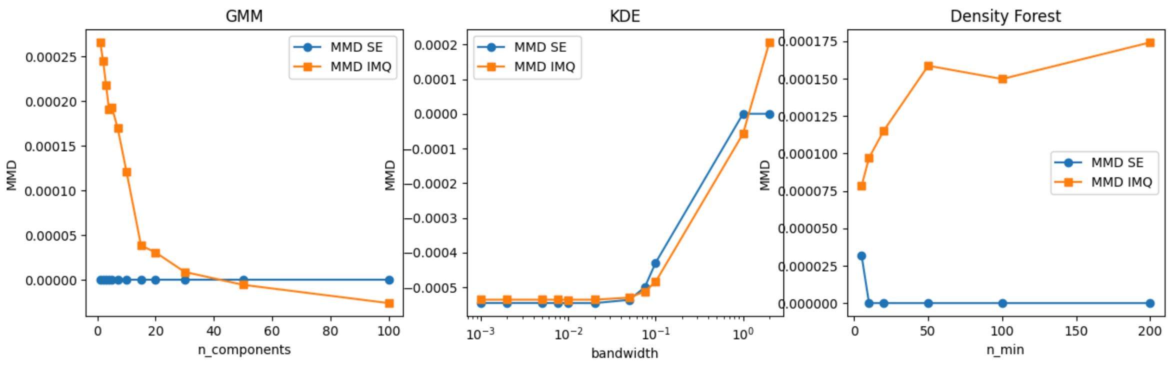

In [161…

```python
# 评估曲线

fig, axes = plt.subplots(1, 3, figsize=(15, 4))

ax = axes[0]
ax.plot(mmd_results['GMM']['parameters'], mmd_results['GMM']['mmd_se'],
ax.plot(mmd_results['GMM']['parameters'], mmd_results['GMM']['mmd_imq'],
ax.set_xlabel('n_components'); ax.set_ylabel('MMD'); ax.set_title('GMM');

ax = axes[1]
ax.plot(mmd_results['KDE']['parameters'], mmd_results['KDE']['mmd_se'],
ax.plot(mmd_results['KDE']['parameters'], mmd_results['KDE']['mmd_imq'],
ax.set_xscale('log'); ax.set_xlabel('bandwidth'); ax.set_ylabel('MMD'); a

ax = axes[2]
ax.plot(mmd_results['DF']['parameters'],  mmd_results['DF']['mmd_se'],
ax.plot(mmd_results['DF']['parameters'],  mmd_results['DF']['mmd_imq'],
ax.set_xlabel('n_min'); ax.set_ylabel('MMD'); ax.set_title('Density Fores
plt.show()
```



Digits is 64-D with pixel values ≈0–16. With the SE kernel and h=1.0, off-diagonal kernel values are ~0, so SE-MMD² stays near zero (tiny negatives are unbiased-estimator noise). The IMQ kernel decays slower, hence it's informative.

GMM:

As n_components increases, flexibility improves → IMQ-MMD² decreases and plateaus. SE stays ~0 due to the bandwidth issue.

KDE:

Very small bandwidth → lowest MMD². Increasing bandwidth oversmooths → IMQ-MMD² rises sharply. SE shows the same trend but compressed near zero.

Density Forest:

Larger n_min → larger leaves → higher bias → IMQ-MMD² increases with n_min. SE remains 0 (same reason).

In [140…

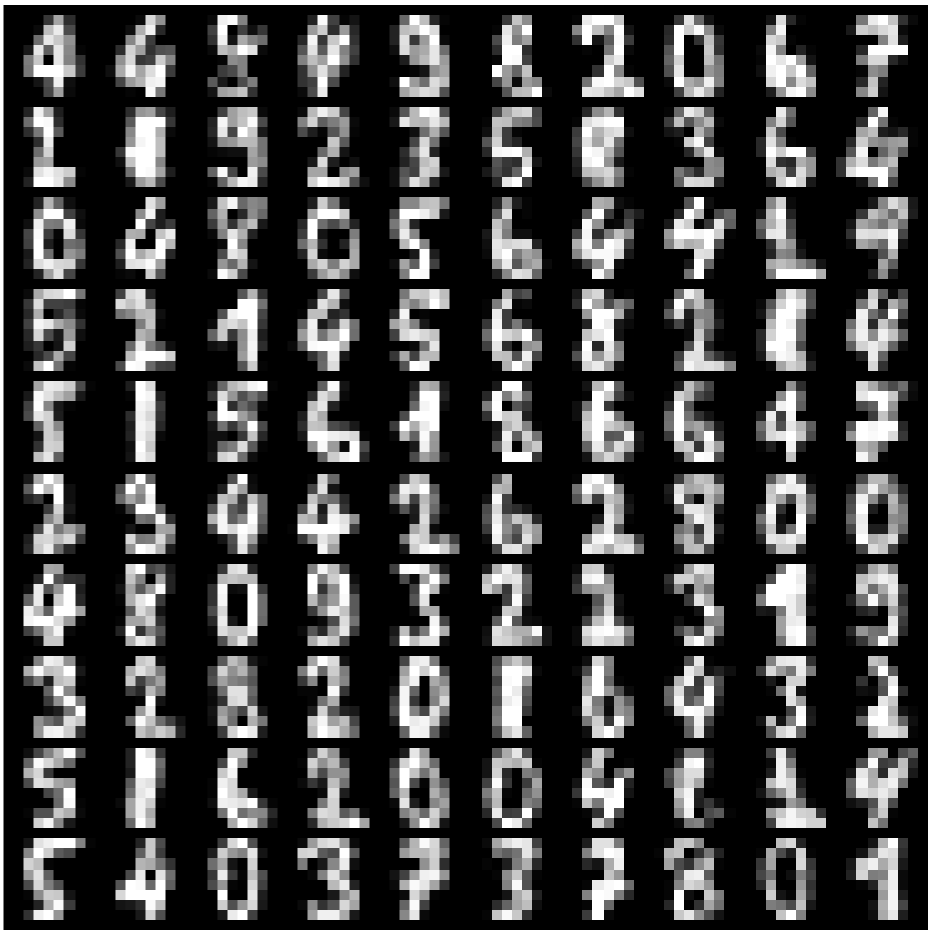
```
def select_models(res, model_name):
    mmd_scores = (np.array(res[model_name]['mmd_se']) + np.array(res[mode
    best_idx = np.argmin(mmd_scores); worst_idx = np.argmax(mmd_scores)
    return (res[model_name]['model'][best_idx], res[model_name]['model'][
            res[model_name]['parameters'][best_idx], res[model_name]['par

gmm_good, gmm_bad, K_good, K_bad = select_models(mmd_results, 'GMM')
kde_good, kde_bad, h_good, h_bad = select_models(mmd_results, 'KDE')
df_good,  df_bad,  nmin_good, nmin_bad = select_models(mmd_results, 'DF')

def gen_samples(model, kind, n=test_size):
    if kind == 'GMM':
        s, _ = model.sample(n); return s
    elif kind == 'KDE':
        return model.sample(n, random_state=42)
    else:
        return model.sample(n)

samples_gmm_good = gen_samples(gmm_good, 'GMM')
samples_gmm_bad  = gen_samples(gmm_bad,  'GMM')
```

```
samples_kde_good = gen_samples(kde_good, 'KDE')
samples_kde_bad  = gen_samples(kde_bad,  'KDE')
samples_df_good  = gen_samples(df_good,  'DF')
samples_df_bad   = gen_samples(df_bad,   'DF')
```

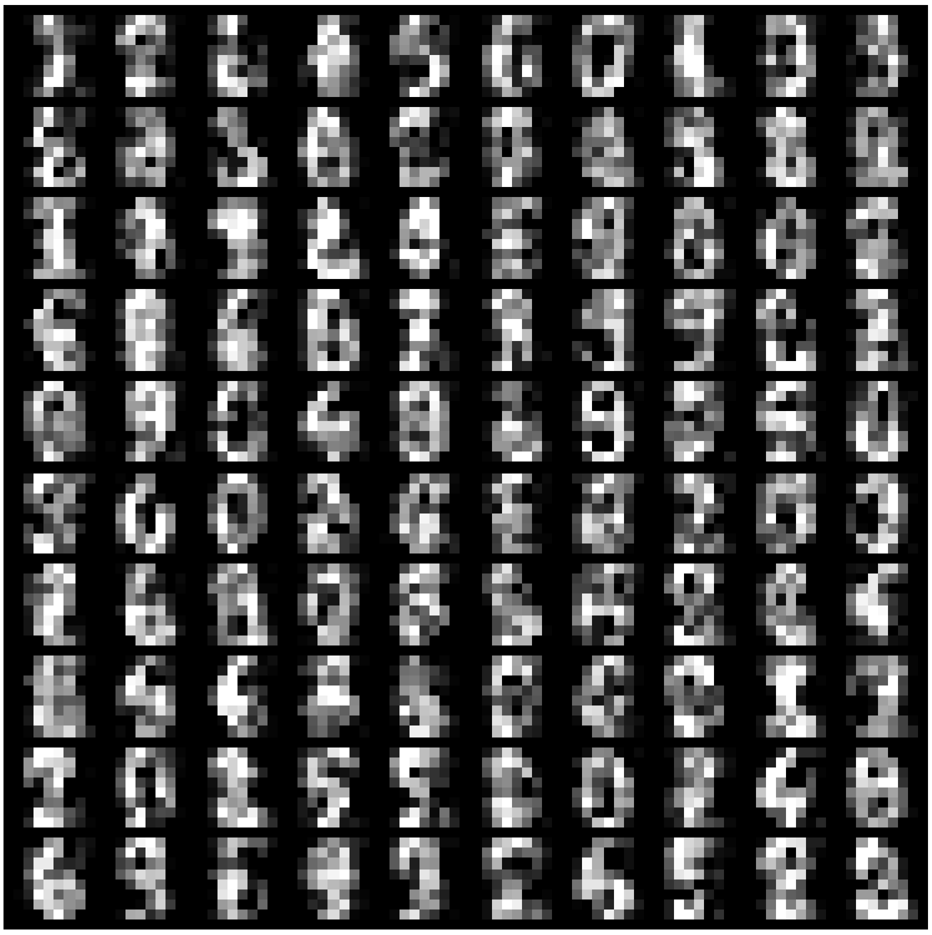
In [141…

```
def show_grid(samples, title, n=10):
    fig, ax = plt.subplots(figsize=(6,6))
    ax.set_title(title); ax.axis('off')
    d = 8
    canvas = np.zeros(((d+1)*n+1, (d+1)*n+1))
    pick = samples.copy()
    rng.shuffle(pick)
    for i in range(n):
        for j in range(n):
            img = pick[i*n + j].reshape(d, d)
            img = np.clip(img, 0, 16)
            canvas[i*(d+1)+1:(i+1)*(d+1), j*(d+1)+1:(j+1)*(d+1)] = img
    ax.imshow(canvas, cmap='gray')
    plt.show()

show_grid(samples_gmm_good, f"GMM good (K={K_good})")
show_grid(samples_gmm_bad,  f"GMM bad  (K={K_bad})")
show_grid(samples_kde_good, f"KDE good (h={h_good})")
show_grid(samples_kde_bad,  f"KDE bad  (h={h_bad})")
show_grid(samples_df_good,  f"DF good  (n_min={nmin_good})")
show_grid(samples_df_bad,   f"DF bad   (n_min={nmin_bad})")
```

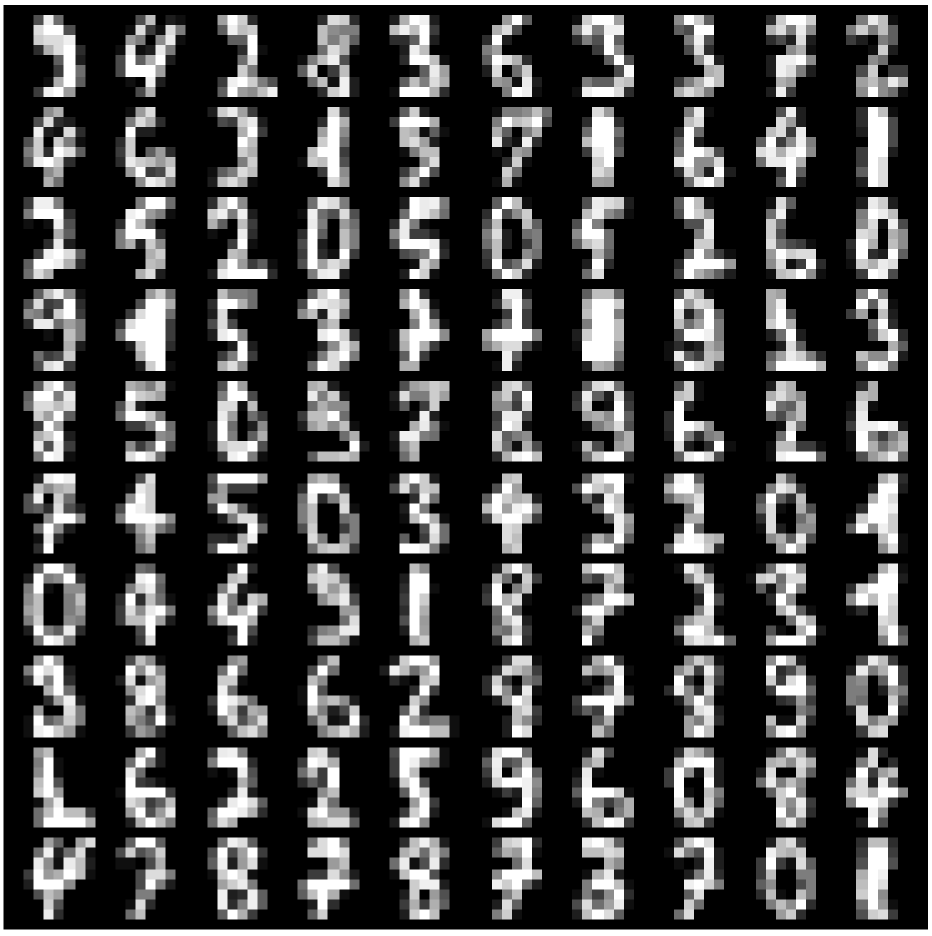
GMM good (K=100)



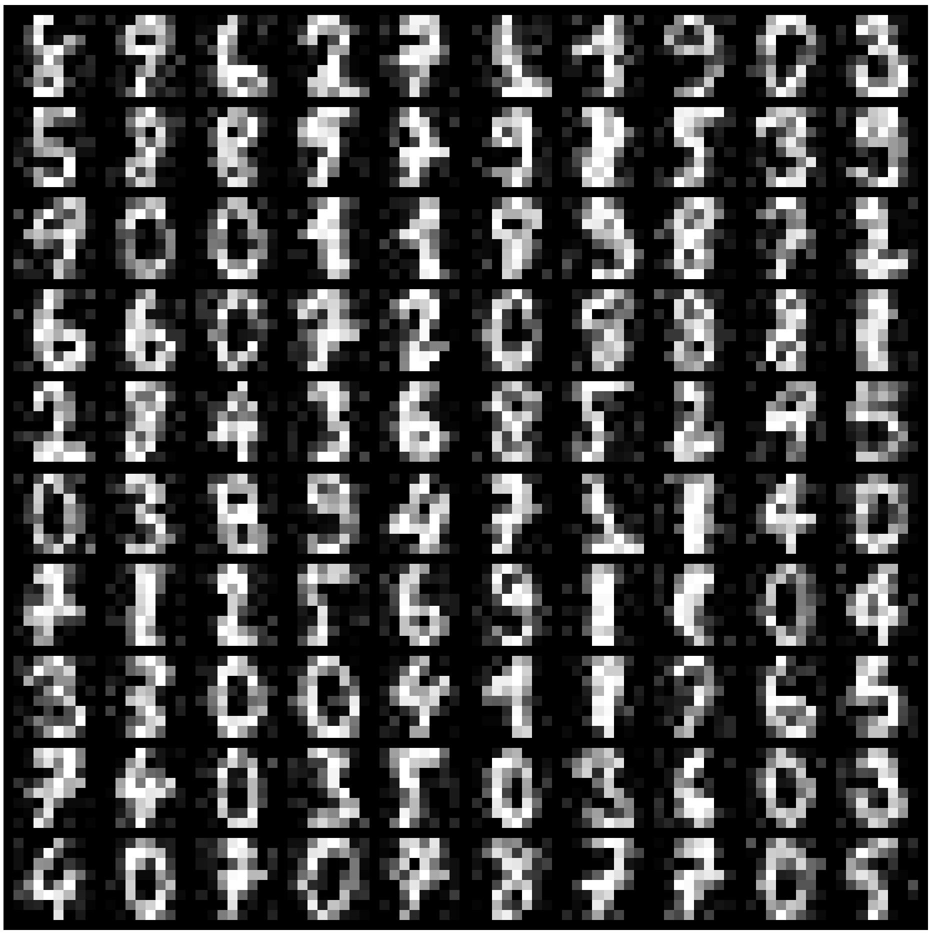
GMM bad (K=1)



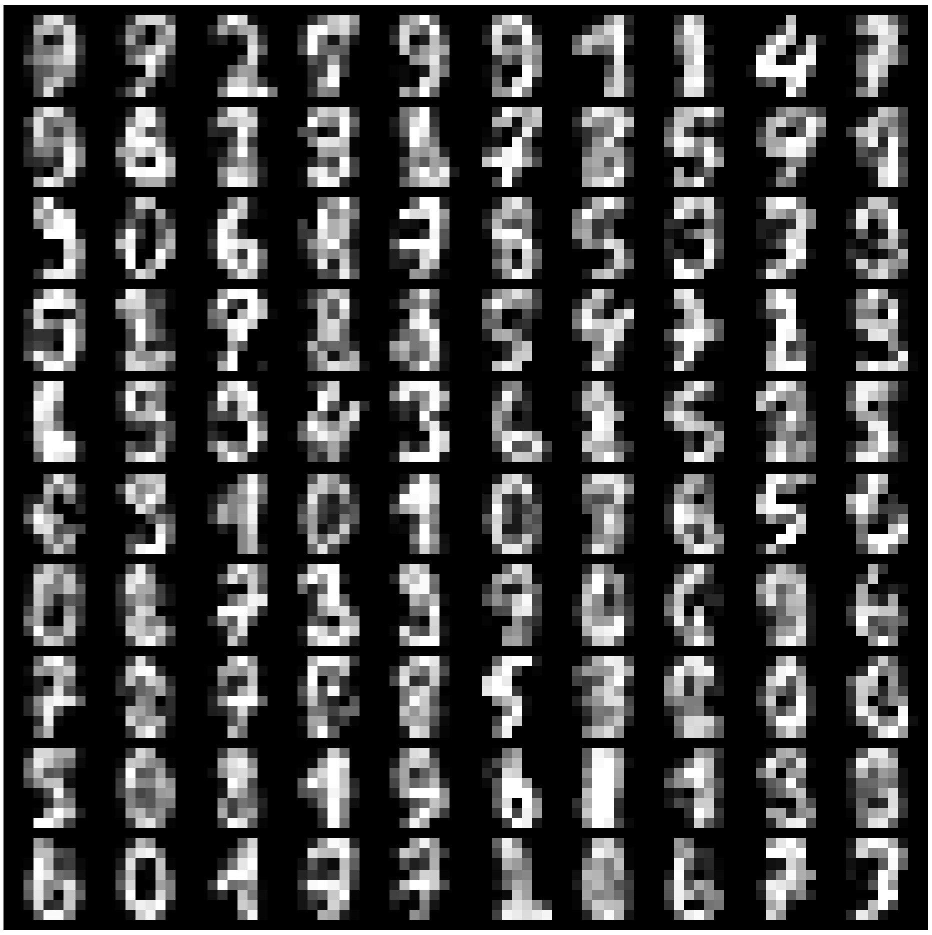
KDE good (h=0.02)



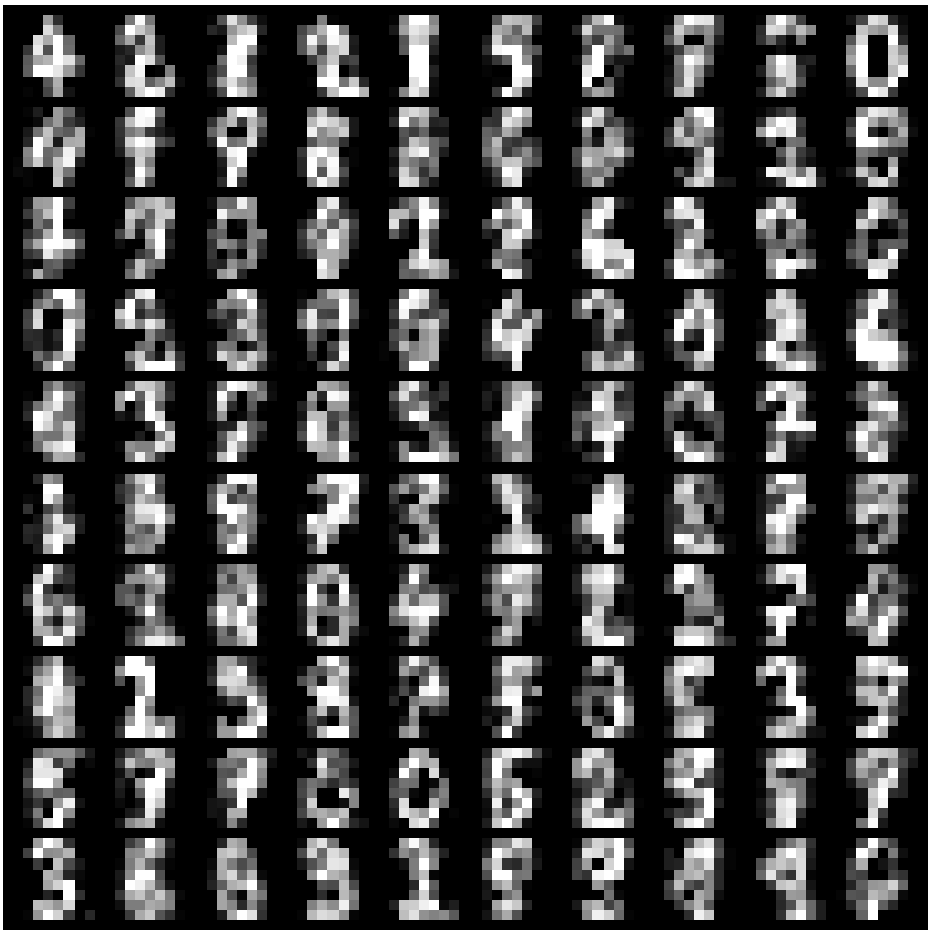
KDE bad (h=2)



DF good (n_min=10)



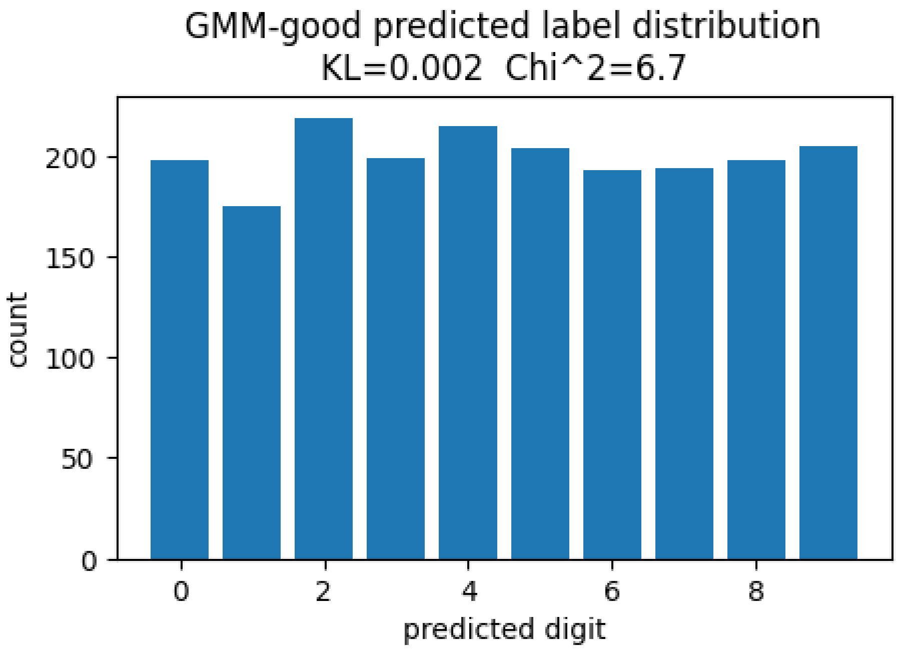
DF bad (n_min=200)

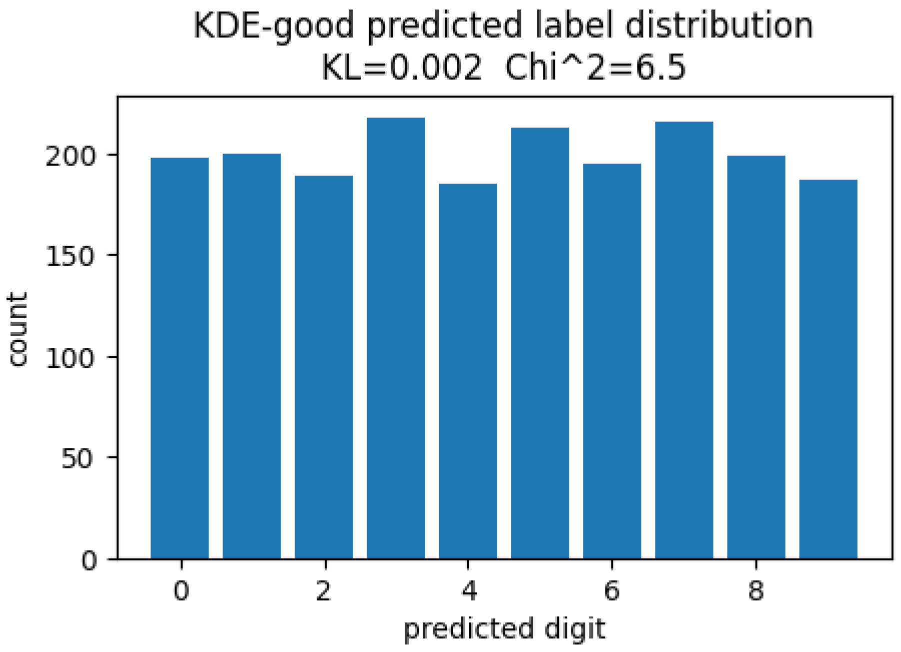


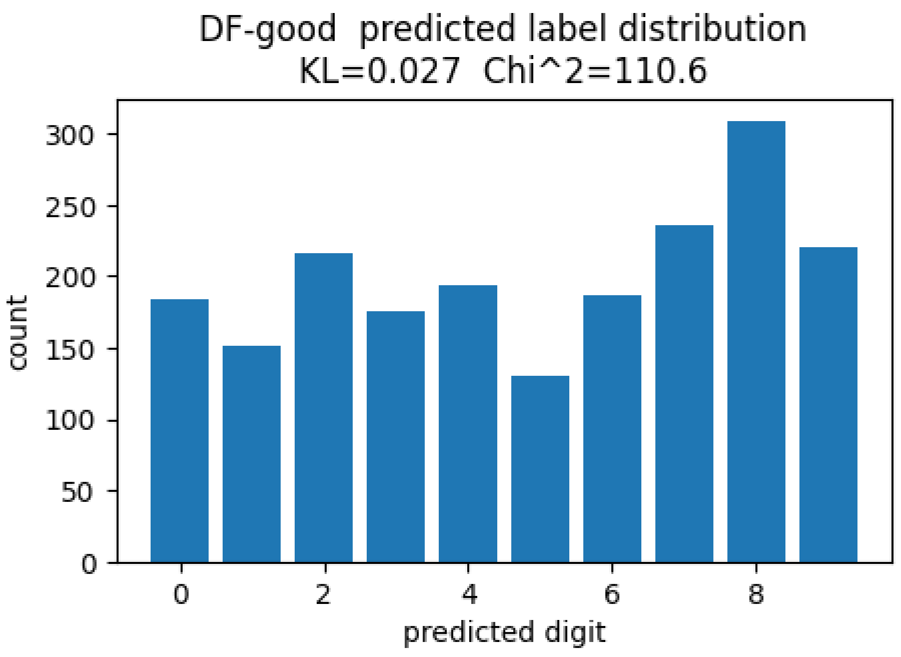
Higher GMM capacity, KDE with a small bandwidth, and DF with small n_min produce sharper, more class-distinct digits, exactly what the IMQ-MMD² curves report. SE-MMD² being near zero is a bandwidthartifact (64-D digits with h=1).

In [142…
```
rf = RandomForestClassifier(n_estimators=200, random_state=42)
rf.fit(X_train, y_train)

def plot_label_hist(pred, title):
    counts = np.bincount(pred, minlength=10)
    p = counts / counts.sum()
    u = np.ones(10)/10
    from scipy.stats import entropy
    kl = entropy(p + 1e-12, u)    # KL(p||uniform)
    chi2 = ((counts - counts.mean())**2 / (counts.mean() + 1e-12)).sum()
    plt.figure(figsize=(5,3))
    plt.bar(range(10), counts)
    plt.title(f"{title}\nKL={kl:.3f}  Chi^2={chi2:.1f}")
    plt.xlabel("predicted digit"); plt.ylabel("count")
    plt.show()
    return counts

pred_gmm = rf.predict(samples_gmm_good)
pred_kde = rf.predict(samples_kde_good)
pred_df  = rf.predict(samples_df_good)

_ = plot_label_hist(pred_gmm, "GMM-good predicted label distribution")
```

```
_ = plot_label_hist(pred_kde, "KDE-good predicted label distribution")
_ = plot_label_hist(pred_df,  "DF-good  predicted label distribution")
```







GMM-good:

Predicted label counts are close to uniform (≈200 per class). KL≈0.002, χ²≈6.7 → essentially balanced and recognisable.

KDE-good:

Also near uniform. KL≈0.002, χ²≈6.5 → balanced and recognisable, consistent with low MMD² at small bandwidth.

DF-good:

Strong class bias (e.g., 8/9 over-represented). KL≈0.027, χ²≈110.6 → clearly not generated in equal proportions, despite recognisable digits.

So, GMM and KDE (with good hyper-parameters) pass the “equal proportions” check; Density Forest does not.

In [ ]:
```
from collections import Counter
def balanced_batch_by_pred(samples,
                           clf,
                           per_class=100,
                           to_clf_space=None,
                           pool_size=None,
                           rng=None):
    """
    samples: 生成样本
    clf:     训练好的分类器（在“分类器空间”训练）
    per_class: 每类要取的样本数
    to_clf_space: 将 samples 映射到“分类器空间”的函数，
                  例如 RF 在原尺度训练而 samples 在 [0,1]，则传 scaler.invers
                  如果本来就在同一尺度，传 None
    pool_size: 先从 samples 里取多少个做候选池；默认用 samples 的全部
    rng:       numpy Random Generator
    """
    rng = np.random.default_rng(0) if rng is None else rng
    # 1) 取候选池
    X_pool = samples if pool_size is None else samples[:pool_size]

    # 2) 映射到分类器空间（很关键！）
    X_for_clf = X_pool if to_clf_space is None else to_clf_space(X_pool)

    # 3) 预测并做分层抽样
    y_pred = clf.predict(X_for_clf)
    counts = Counter(y_pred.tolist())
    if len(counts) < 2:
        raise ValueError(f"All samples predicted as one class: {counts}.
                         f"Check scaling: to_clf_space={to_clf_space is n

    idxs = []
    for c in range(10):
        pool = np.where(y_pred == c)[0]
        if len(pool) == 0:
            continue
        take = rng.choice(pool, size=per_class, replace=(len(pool) < per_
        idxs.append(take)
    if not idxs:
        raise ValueError("No classes available for balancing. Check input
    idxs = np.concatenate(idxs)

    # 返回分类器空间的样本（注意：这里返回的是“分类器空间”的样本）
    return X_for_clf[idxs], y_pred[idxs], counts

rf = RandomForestClassifier(n_estimators=200, random_state=42).fit(X_trai
bal_gmm, yb_gmm, cnt = balanced_batch_by_pred(samples_gmm_good, rf, per_c
bal_kde, yb_kde, cnt = balanced_batch_by_pred(samples_kde_good, rf, per_c
bal_df,  yb_df, cnt  = balanced_batch_by_pred(samples_df_good,  rf, per_c
```

In [152…

```
def show_grid_with_labels(samples, preds, title, n=10, vmax=16):
    import matplotlib.pyplot as plt
    d = 8
    fig, axes = plt.subplots(n, n, figsize=(8, 6)); fig.suptitle(title)
    for i in range(n):
        for j in range(n):
            k = i*n + j
            axes[i,j].imshow(np.clip(samples[k].reshape(d,d), 0, vmax),
                             cmap='gray', vmin=0, vmax=vmax)
            axes[i,j].axis('off')
            axes[i,j].text(1.25, 0.15, str(preds[k]), fontsize=12, color=
                           transform=axes[i,j].transAxes, ha='center', va
    plt.show()
```

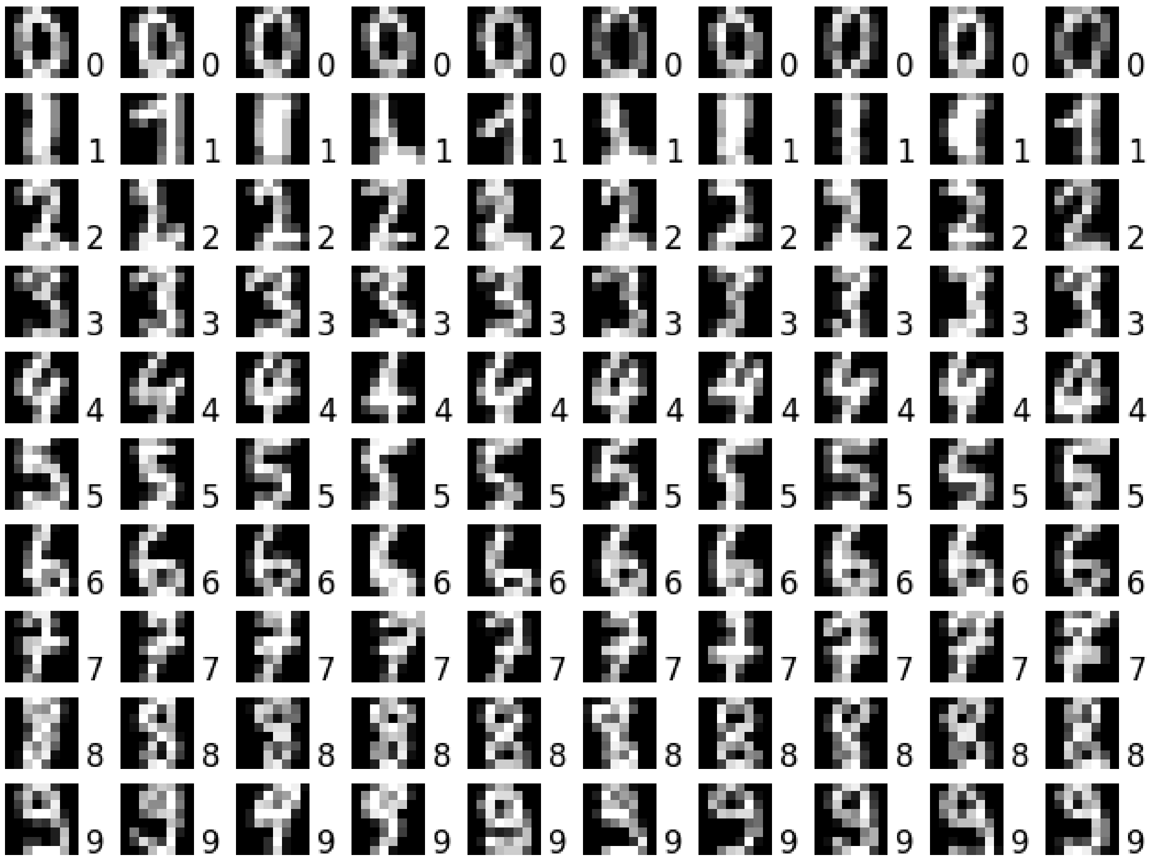
In [153…

```
if len(bal_gmm): show_grid_with_labels(bal_gmm, yb_gmm, "GMM-good — balan
if len(bal_kde): show_grid_with_labels(bal_kde, yb_kde, "KDE-good — balan
if len(bal_df):  show_grid_with_labels(bal_df,  yb_df,  "DF-good  — balan
```

GMM-good — balanced 10× classes

0
1
2
3
4
5
6
7
8
9

KDE-good — balanced 10× classes



DF-good — balanced 10× classes

0
1
2
3
4
5
6
7
8
9