Meta OT and Sinkhorn Initializers

Contents

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This tutorial covers how to learn a Meta OT initializer for Sinkhorn from Amos et al., 2022 to help predict a reasonable starting point, and along the way we will also consider the Gaussian initializer from Thornton and Cuturi, 2022. These initialization schemes can greatly improve the convergence of Sinkhorn's algorithm, which otherwise usually starts from a zero initialization. Deploying optimal transport methods often involve needing to solve many similar OT problems. While Sinkhorn can be run independently on the problems to solve them from scratch, Meta OT methods argue that the runtime of the solver can be significantly improved by learning about the shared structure between the problem instances and using it to predict an approximate starting point that can be further refined.

We will cover:

- ott.core.initializers.MetaOTInitializer: The main class for the Meta OT initializer
- ott.core.initializers.Meta_MLP: A Meta MLP to predict the dual potentials from the weights of the measures.
- ott.core.initializers.GaussianInitializer: The main initialization class for the Gasusian initializer

[1]:
```
from ott.geometry import pointcloud
from ott.core import initializers as init_lib
from ott.core import linear_problems, sinkhorn

import jax
from jax import numpy as jnp

import numpy as np
from collections import namedtuple
import torchvision

import matplotlib.pyplot as plt
from matplotlib import cm
```

[2]:
```
# Obtain the MNIST dataset and flatten the images into discrete measures.
def get_mnist_flat(train):
    dataset = torchvision.datasets.MNIST(
        "/tmp/mnist/",
        download=True,
        train=train,
    )
    data = jnp.array(dataset.data)
    data = data / 255.0
    data = data.reshape(-1, 784)
    data = data / data.sum(axis=1, keepdims=True)
    return data


mnist_train_data = get_mnist_flat(True)
mnist_eval_data = get_mnist_flat(False)

# Set up the geometry to use the grid of pixels
sinkhorn_epsilon = 1e-2
x_grid = []
for i in jnp.linspace(1, 0, num=28):
    for j in jnp.linspace(0, 1, num=28):
        x_grid.append([j, i])
x_grid = jnp.array(x_grid)
geom = pointcloud.PointCloud(x=x_grid, y=x_grid, epsilon=sinkhorn_epsilon)

# Sample pairs of flattened MNIST digits
OT_Pair = namedtuple("OT_Pair", "a b")


def sample_OT_pairs(key, batch_size=128, train=True):
    data = mnist_train_data if train else mnist_eval_data
    k1, k2, key = jax.random.split(key, num=3)
    I = jax.random.randint(k1, shape=[batch_size], minval=0,
maxval=len(data))
    J = jax.random.randint(k2, shape=[batch_size], minval=0,
maxval=len(data))
    a = data[I]
    b = data[J]
    return OT_Pair(a, b)


# Generate an interpolation between the measures by sampling from the
transport map.
def interpolate(
    key,
    f,
    g,
    a,
    b,
    num_interp_frames=8,
    title=None,
    axs=None,
    num_estimation_iterations=20,
    num_samples_marginal=1000,
):
    P = geom.transport_from_potentials(f, g)
    log_P_flat = jnp.log(P).ravel()

    @jax.jit
    def sample_interp_histogram_single(key, t):
        map_samples = jax.random.categorical(
            key, logits=log_P_flat, shape=[num_samples_marginal]
        )
        a_samples = geom.x[map_samples // len(a)]
        b_samples = geom.y[map_samples % len(a)]
        interp_samples = (1.0 - t) * a_samples + t * b_samples
        interp_hist, _, _ = jnp.histogram2d(
            interp_samples[:, 1],
            interp_samples[:, 0],
            bins=jnp.linspace(0.0, 1.0, num=28 + 1),
        )
        interp_hist = jnp.flipud(interp_hist)
        return interp_hist

    def sample_interp_histogram(key, t):
        alpha_t = 0.0
        for _ in range(num_estimation_iterations):
            k1, key = jax.random.split(key)
            alpha_t += sample_interp_histogram_single(k1, t)
        alpha_t = np.array(alpha_t)
        thresh = np.quantile(alpha_t, 0.95)
        alpha_t[alpha_t > thresh] = thresh
        return alpha_t / alpha_t.max()

    if axs is None:
        nrow, ncol = 1, num_interp_frames
        fig, axs = plt.subplots(
            nrow,
            ncol,
            figsize=(1 * ncol, 1 * nrow),
            gridspec_kw={"wspace": 0, "hspace": 0},
            dpi=80,
        )

    for i, t in enumerate(jnp.linspace(0, 1, num=num_interp_frames)):
        k1, key = jax.random.split(key)
        alpha_t = sample_interp_histogram(k1, t)
        axs[i].imshow(alpha_t.reshape(28, 28), cmap=cm.Greys)

    for ax in axs:
        ax.set_xticks([])
        ax.set_yticks([])

    if title is not None:
        fig.suptitle(title, y=1.2, fontsize=20)
```

Computing the optimal transport map between images provides a way of connecting their pixel intensities. For example, Cuturi, 2013 uses the OT distance between MNIST digits for classification, which we will focus on in this tutorial.

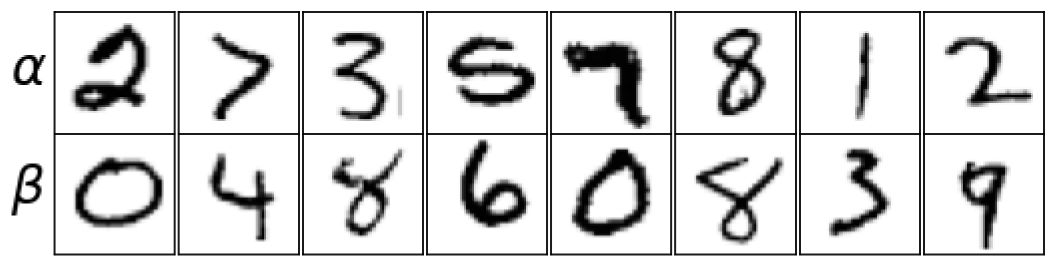
Transporting between paris of MNIST digits is a setting where the OT map needs to be repeatedly computed between every pair of digits. The standard use of optimal transport for solving these coupling problems is to treat every problem independently and solve each one from scratch. This is inefficient as similar problem instances, especially between similar digits, have similar solutions and transport maps.

Meta OT [Amos et al., 2022] is a way of learning this shared structure. This tutorial shows how to train a meta OT model to predict the optimal Sinkhorn potentials from the image pairs. We will reproduce their results using OTT's Meta OT initializer, which provides an easy-to-use interface for training and using Meta OT models.

We consider each MNIST digit (a 28x28 grayscale image) as a discrete distribution with fixed support as pixel coordinates and the weights are the normalized pixel intensity values corresponding to the pixel coordinate for each digit. Hence, x and y correspond to pixel coordinates, and each digit corresponds to a discrete distribition with support of size $n_a = n_b = 28 \cdot 28 = 784$.

The next block shows how our sampling function can be used to obtain batches of pairs of MNIST evaluation images.

```
[3]: key = jax.random.PRNGKey(0)
     num_samples = 8
     demo_batch = sample_OT_pairs(key, batch_size=num_samples, train=False)

     nrow, ncol = 2, num_samples
     fig, axs = plt.subplots(
         nrow,
         ncol,
         figsize=(1 * ncol, 1 * nrow),
         gridspec_kw={"wspace": 0, "hspace": 0},
         dpi=80,
     )

     for batch_idx in range(ncol):
         axs[0, batch_idx].imshow(
             demo_batch.a[batch_idx].reshape(28, 28), cmap=cm.Greys
         )
         axs[1, batch_idx].imshow(
             demo_batch.b[batch_idx].reshape(28, 28), cmap=cm.Greys
         )

     for ax in axs.ravel():
         ax.set_xticklabels([])
         ax.set_yticklabels([])
         ax.set_xticks([])
         ax.set_yticks([])
     axs[0, 0].set_ylabel(r"$\alpha$", rotation=0, size=24)
     axs[0, 0].yaxis.set_label_coords(-0.2, 0.3)
     axs[1, 0].set_ylabel(r"$\beta$", rotation=0, size=24)
     axs[1, 0].yaxis.set_label_coords(-0.2, 0.3)
```



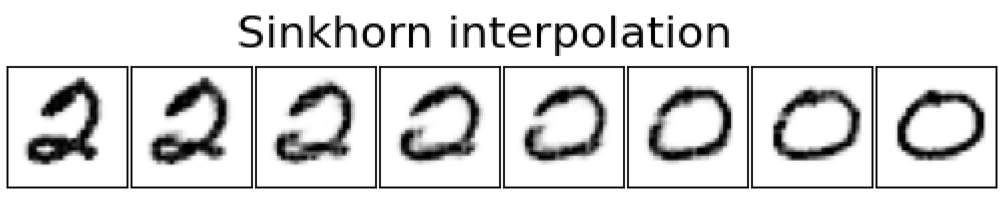
We interpret the pair of MNIST digits as discrete measures $\alpha = \sum_{i=1}^{n_a} a_i \delta_{x_i}$ and $\beta = \sum_{j=1}^{n_b} b_j \delta_{y_j}$. The default Sinkhorn implementation in ott.core.sinkhorn.sinkhorn can easily compute their optimal coupling from scratch. The iterates are the dual potentials, f and g, and Sinkhorn iteratively improves them to find them. The optimal transport map and an interpolation between the measures can be computed from these optimal dual potentials.

This next block solves the discrete OT problem associated with the first instance of the batch above with `sinkhorn` and visualizes the OT interpolation. Given the optimal transport map $P^\star$, the interpolation shows

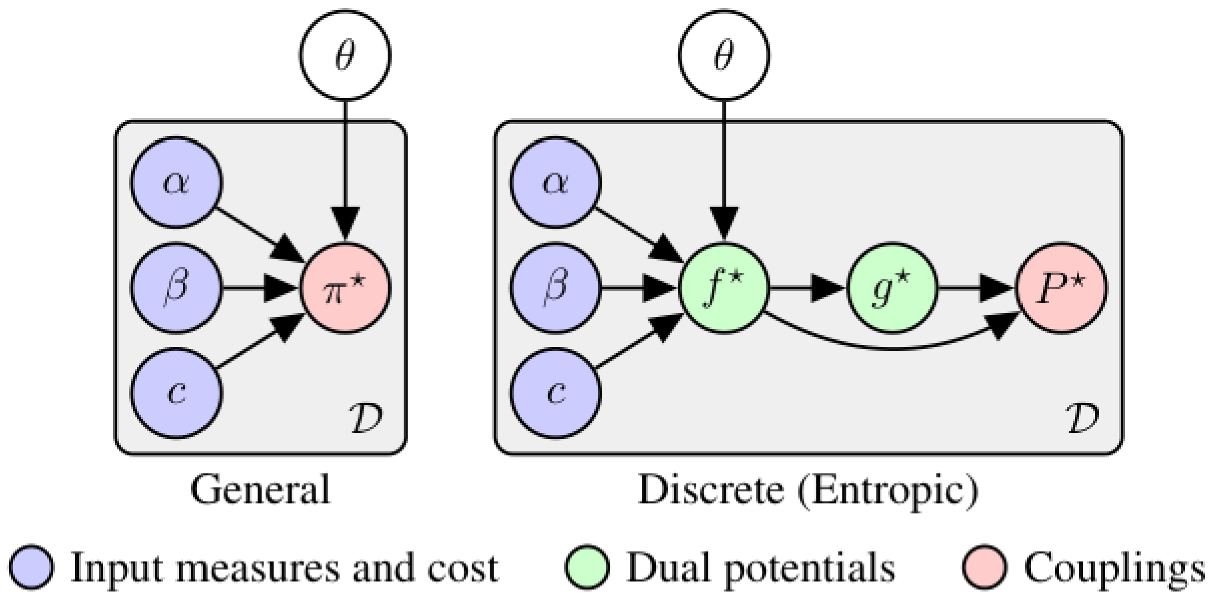
$$\alpha_t = (t\mathrm{proj}_y + (1-t)\mathrm{proj}_x)_\# P^\star$$

where $t \in [0,1]$, $\mathrm{proj}_x(x,y) := x$, and $\mathrm{proj}_y(x,y) := y$.

```
[4]: a, b = demo_batch.a[0], demo_batch.b[0]
base_sink_out = sinkhorn.sinkhorn(geom, a=a, b=b)
interpolate(
    key, base_sink_out.f, base_sink_out.g, a, b, title="Sinkhorn
interpolation"
)
```



For discrete OT, Meta OT (Amos et al., 2022) predicts the optimal dual variables $f^\star$ from the input measures α, β and geometry, which can then map to $g^\star$ and the transport map $P^\star$:



We will consider a model $\hat{f}_\theta(a,b)$ that predicts the duals given the probabilities of the measures, i.e. a and b, leaving the geometry (and cost) fixed. The MNIST measures fit into this setting because the pixel locations remain fixed.

Learning the model. The goal is for the model to match the optimal duals, i.e., $\hat{f}_\theta \approx f^\star$. This can be done by training the predictions of f_θ to optimize the dual objective, which $f^\star$ also optimizes for. The overall learning setup can thus be written as:

$$\min_\theta \; \mathbb{E}_{(\alpha,\beta)\sim\mathcal{D}} \; J(\hat{f}_\theta(a,b); \alpha, \beta),$$

where a, b are the probabilities of the measures α, β, $\mathcal{D}$ is some distribution of optimal transport problems, and

$$-J(f; \alpha, \beta, c) := \langle f, a\rangle + \langle g, b\rangle - \epsilon \left\langle \exp\{f/\epsilon\}, K \exp\{g/\epsilon\}\right\rangle$$

is the entropic dual objective, and $K_{i,j} := -C_{i,j}/\epsilon$ is the *Gibbs kernel*. Notably, this loss **doesn't require access to the ground-truth** $f^\star$ and instead locally updates the predictions. In other words, the Meta OT model simultaneously solves all of the OT problems in the meta distribution $\mathcal{D}$ during training.

The following instantiates ott.core.initializers.MetaOTInitializer, which provides an implementation for training and deploying Meta OT models. The default meta potential model for f_θ is a standard multi-layer MLP defined in ott.core.initializers.Meta_MLP and it is optimized with Adam by default.

Custom model and optimizers. The model and training procedure use flax and optax. The Meta OT initializer can take a custom-written Flax module in `init_model` or optimizer in `opt` that may be better-suited to your setting than an MLP.

We can create the initializer by providing it with the shared geometry of the problem instances.

```
[5]: meta_initializer = init_lib.MetaOTInitializer(geom=geom)
```

Meta OT models have a preliminary training phase where they are given samples of OT problems from the meta distribution. The Meta OTT initializer internally stores the training state of the model, and `update_fn` will update the initialization on a batch of problems to improve the next prediction. While we show here a separate training phase, the update can also be done in-tandem with deployment where the initialization is then used with a Sinkhorn refinement process to obtain optimal solutions. This is appealing for deployment settings because even if the Meta OT model is suboptimal, refining the prediction with Sinkhorn is **guaranteed** to provide an optimal solution to the transport problem.

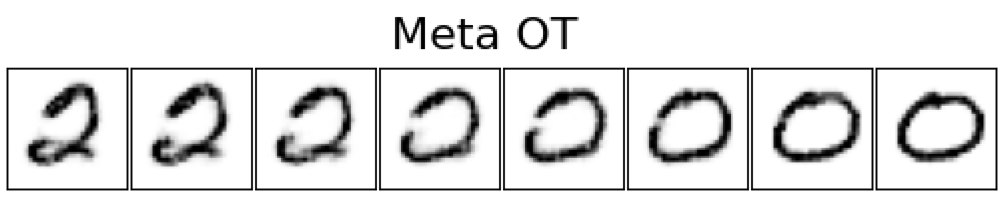
```
[6]: num_train_iterations = 50000

     for train_iter in range(num_train_iterations):
         key, step_key = jax.random.split(key)
         batch = sample_OT_pairs(step_key, train=True)
         loss, init_f, meta_initializer.state = meta_initializer.update(
             meta_initializer.state, a=batch.a, b=batch.b
         )
         print(f"Train iteration: {train_iter+1} - Loss: {loss:.2e}", end="\r")
```

```
Train iteration: 50000 - Loss: -3.54e-02
```

Now that we have trained the model, we can next deploy it anytime we want to make a rough predition for new instances of the problems. While in practice, the model can be continued to be updated in deployment by calling `update`, here we will keep the model fixed so we can evaluate it on test instances.

We can visualize the interpolation provided by the Meta OT model's prediction of the solution to the transport problems from above, which are sampled from testing pairs of MNIST digits that the model was not trained on. The initializer uses the Meta OT model in `init_dual_a`. This shows that the initialization is extremely close to the ground-truth coupling.

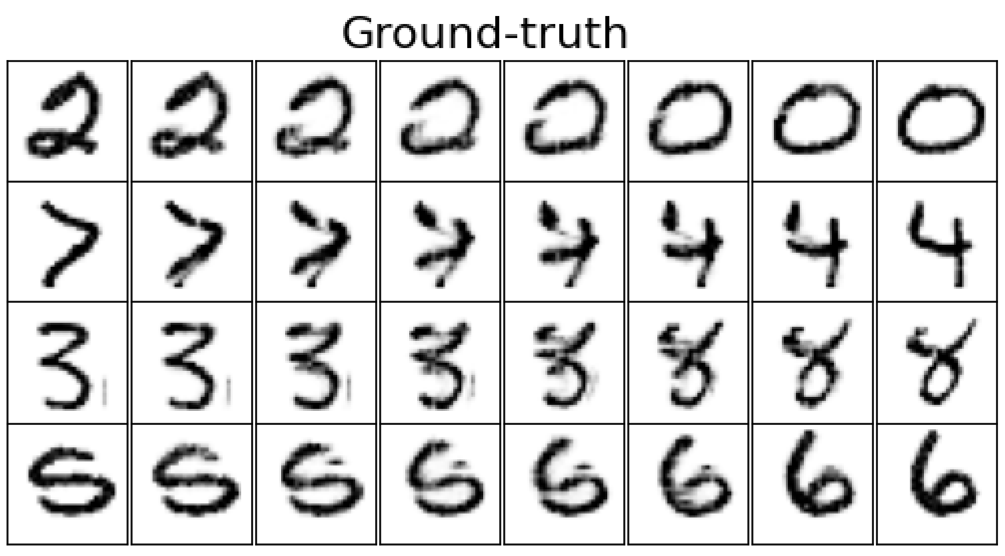
```
[7]: a, b = demo_batch.a[0], demo_batch.b[0]
     ot_problem = linear_problems.LinearProblem(geom, a, b)

     # Predict the optimal f duals.
     f = meta_initializer.init_dual_a(ot_problem, lse_mode=True)

     # Obtain the optimal g duals from the prediction.
     g = geom.update_potential(f, jnp.zeros_like(b), jnp.log(b), 0, axis=0)

     interpolate(key, f, g, a, b, title="Meta OT")
```

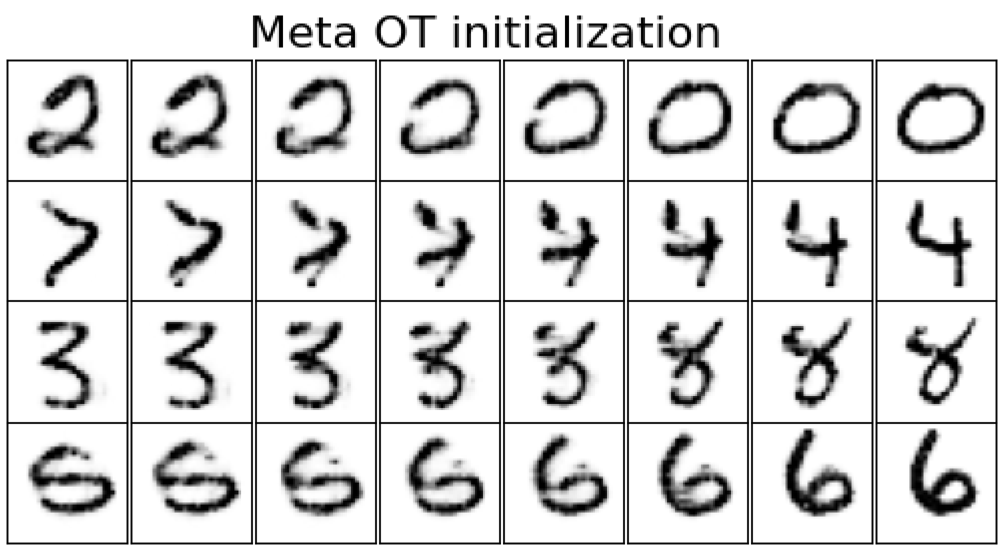


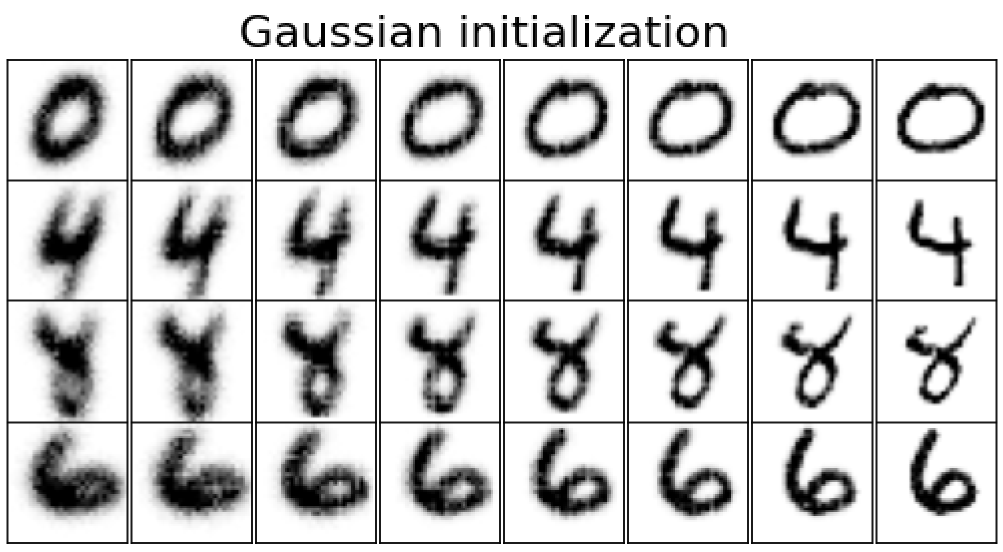
We next visualize the initializations on a few other instances from the problems from above, comparing:

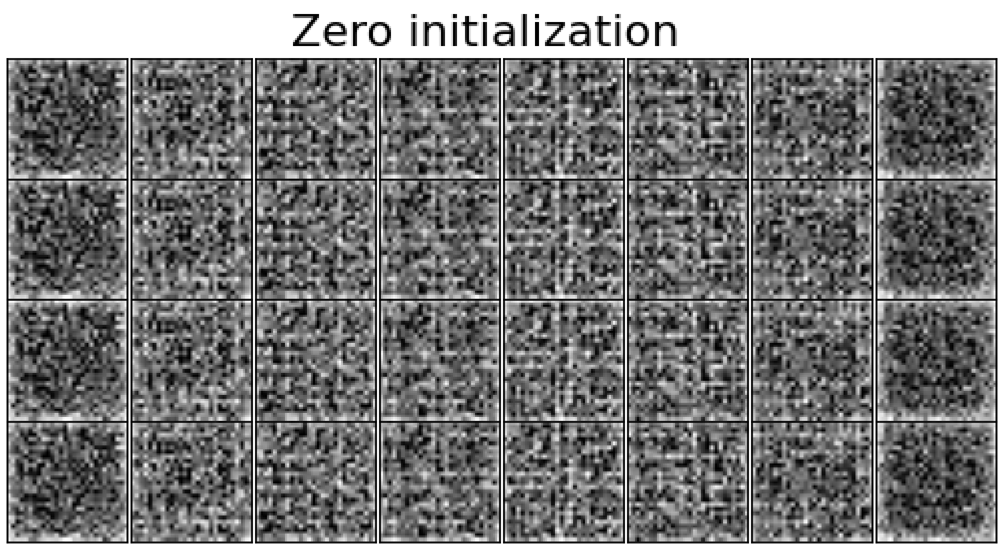
1. the ground-truth solution obtained from Sinkhorn,
2. Meta OT's prediction,
3. the Gaussian initialization from Thornton and Cuturi, 2022, and
4. the default initialization of $f = 0$.

[8]:
```
def plot_demo_initializations(
    get_potentials, title, num_interp_frames=8, num_pairs=4
):
    nrow, ncol = num_pairs, num_interp_frames
    fig, axs = plt.subplots(
        nrow,
        ncol,
        figsize=(1 * ncol, 1 * nrow),
        gridspec_kw={"wspace": 0, "hspace": 0},
        dpi=80,
    )
    fig.suptitle(title, y=0.95, fontsize=20)
    for i in range(num_pairs):
        a, b = demo_batch.a[i], demo_batch.b[i]
        f, g = get_potentials(a, b)
        interpolate(key, f, g, a, b, axs=axs[i, :])


def get_sinkhorn_potentials(a, b):
    base_sink_out = sinkhorn.sinkhorn(geom, a=a, b=b)
    return base_sink_out.f, base_sink_out.g


plot_demo_initializations(get_sinkhorn_potentials, title="Ground-truth")


def get_meta_ot_potentials(a, b):
    ot_problem = linear_problems.LinearProblem(geom, a, b)
    f = meta_initializer.init_dual_a(ot_problem, lse_mode=True)
    g = geom.update_potential(f, jnp.zeros_like(b), jnp.log(b), 0, axis=0)
    return f, g


plot_demo_initializations(
    get_meta_ot_potentials, title="Meta OT initialization"
)


def get_gaussian_potentials(a, b):
    ot_problem = linear_problems.LinearProblem(geom, a=a, b=b)
    f = init_lib.GaussianInitializer().init_dual_a(ot_problem,
lse_mode=True)
    g = geom.update_potential(f, jnp.zeros_like(b), jnp.log(b), 0, axis=0)
    return f, g


plot_demo_initializations(
    get_gaussian_potentials, title="Gaussian initialization"
)


def get_zero_potentials(a, b):
    return jnp.zeros_like(base_sink_out.f), jnp.zeros_like(base_sink_out.g)


plot_demo_initializations(get_zero_potentials, title="Zero initialization")
```







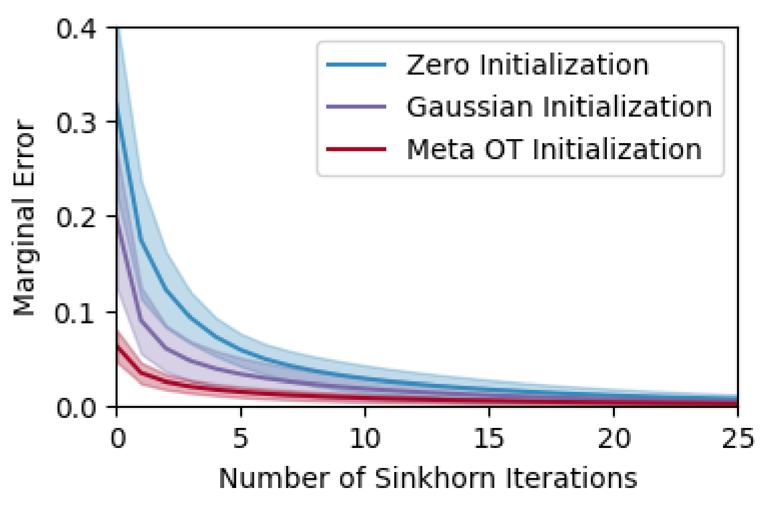


We lastly compare how much the initializers help Sinkhorn converge on these problems, measured by the marginal error:

$$\mathrm{err}(f, g; \alpha, \beta, c) := \|P1_m - a\|_1 + \|P^\top 1_n - b\|_1$$

[9]:
```python
def get_errors(sink_out):
    return sink_out.errors[sink_out.errors > -1]


error_log = {"gaus": [], "base": [], "meta_ot": []}

num_evals = 10
eval_batch = sample_OT_pairs(
    jax.random.PRNGKey(0), batch_size=num_evals, train=False
)
for i in range(num_evals):
    a = eval_batch.a[i]
    b = eval_batch.b[i]

    sink_kwargs = {
        "jit": True,
        "threshold": -1,
        "inner_iterations": 1,
        "max_iterations": 26,
    }

    ot_problem = linear_problems.LinearProblem(geom, a=a, b=b)
    base_sink_out = sinkhorn.sinkhorn(
        geom, a=a, b=b, init_dual_a=None, **sink_kwargs
    )

    init_dual_a = meta_initializer.init_dual_a(ot_problem, lse_mode=True)
    meta_sink_out = sinkhorn.sinkhorn(
        geom, a=a, b=b, init_dual_a=init_dual_a, **sink_kwargs
    )

    init_dual_a = init_lib.GaussianInitializer().init_dual_a(
        ot_problem, lse_mode=True
    )
    gaus_sink_out = sinkhorn.sinkhorn(
        geom, a=a, b=b, init_dual_a=init_dual_a, **sink_kwargs
    )

    error_log["base"].append(base_sink_out.errors)
    error_log["meta_ot"].append(meta_sink_out.errors)
    error_log["gaus"].append(gaus_sink_out.errors)

error_log = {key: jnp.array(errors) for (key, errors) in error_log.items()}
```

```
[10]: fig, ax = plt.subplots(figsize=(4, 2.5), dpi=100)
tag_map = {
    "meta_ot": "Meta OT Initialization",
    "gaus": "Gaussian Initialization",
    "base": "Zero Initialization",
}

bmh_colors = plt.style.library["bmh"]["axes.prop_cycle"].by_key()["color"]
colors = [bmh_colors[0], bmh_colors[2], bmh_colors[1]]
for tag, color in zip(["base", "gaus", "meta_ot"], colors):
    mean_errors = jnp.mean(error_log[tag], axis=0)
    ax.plot(mean_errors, label=tag_map[tag], color=color)

    iters = np.arange(len(mean_errors))
    stds = jnp.std(error_log[tag], axis=0)
    ax.fill_between(
        iters, mean_errors - stds, mean_errors + stds, color=color,
alpha=0.3
    )

ax.set_xlabel("Number of Sinkhorn Iterations")
ax.set_ylabel("Marginal Error")
ax.legend()
ax.set_xlim(0, 25)
ax.set_ylim(0, 0.4);
```


Zero Initialization
Gaussian Initialization
Meta OT Initialization
Marginal Error
Number of Sinkhorn Iterations