Transport Cost

$$\texttt{TransportCost}(\texttt{Rectify}(\{X_t\})) \leq \texttt{TransportCost}(\{X_t\}).$$

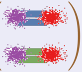
Key Property: Transport Cost

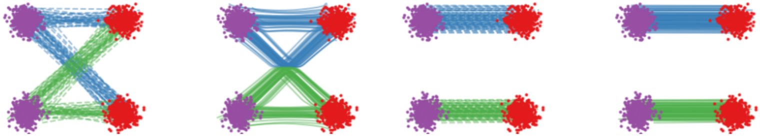
Rectified Flow reduces all convex transport costs

If $\{Z_t\} = \texttt{Rectify}(\{X_t\})$, then

$$\mathbb{E}\left[c(Z_1 - Z_0)\right] \leq \mathbb{E}\left[c(X_1 - X_0)\right], \quad \text{for all convex functions } c$$

Intuition: Untangling Crossings Reduces Transport Cost

$\mathbb{E}\left[\|X_0 - X_1\|\right] = \text{Length}\Big($  $\Big) = \text{Length}\Big($  $\Big) \geq \text{Length}\Big($  $\Big) = \mathbb{E}\left[\|Z_0 - Z_1\|\right],$



Key Property: Rectified Flow Reduces Transport Cost

- **Reducing Transport Cost**:

$$\mathbb{E}\left[c(Z_1 - Z_0)\right] \le \mathbb{E}\left[c(X_1 - X_0)\right], \quad \text{for all convex functions } c$$

Proof

Apply Jensen's inequality + marginal preservation.

$$
\begin{aligned}
\mathbb{E}\left[c(Z_1 - Z_0)\right] &= \mathbb{E}\left[c\left(\int_0^1 v^X(Z_t, t)\mathrm{d}t\right)\right] && \text{//as } \mathrm{d}Z_t = v^X(Z_t, t)\mathrm{d}t \\
&\le \mathbb{E}\left[\int_0^1 c\left(v^X(Z_t, t)\right)\mathrm{d}t\right] && \text{//convexity of } c\text{, Jensen's inequality} \\
&= \mathbb{E}\left[\int_0^1 c\left(v^X(X_t, t)\right)\mathrm{d}t\right] && \text{//} X_t \text{ and } Z_t \text{ shares the same marginals} \\
&= \mathbb{E}\left[\int_0^1 c\left(\mathbb{E}\left[(X_1 - X_0) \mid X_t\right]\right)\mathrm{d}t\right] && \text{//definition of } v^X \\
&\le \mathbb{E}\left[\int_0^1 \mathbb{E}\left[c\left(X_1 - X_0\right) \mid X_t\right]\mathrm{d}t\right] && \text{//convexity of } c\text{, Jensen's inequality} \\
&= \int_0^1 \mathbb{E}\left[c\left(X_1 - X_0\right)\right]\mathrm{d}t && \text{//}\mathbb{E}\left[\mathbb{E}\left[(X_1 - X_0)|X_t\right]\right] = \mathbb{E}\left[(X_1 - X_0)\right] \\
&= \mathbb{E}\left[c\left(X_1 - X_0\right)\right].
\end{aligned}
$$

Key Property: Rectified Flow Reduces Transport Cost

- **Reducing Transport Cost**:

$$\mathbb{E}\left[c(Z_1 - Z_0)\right] \leq \mathbb{E}\left[c(X_1 - X_0)\right], \qquad \text{for all convex functions } c$$

Proof

Key: averaging the slope $\dot{X}_t$ given X_t reduces the transport cost:

$$\begin{aligned}
\int_0^1 \mathbb{E}\left[c\left(\dot{X}_t\right)\right] \mathrm{d}t &= \int_0^1 \mathbb{E}\left[\mathbb{E}\left[c\left(\dot{X}_t\right) \mid X_t\right]\right] \mathrm{d}t \\
&\geq \int_0^1 \mathbb{E}\left[c\left(\mathbb{E}\left[\dot{X}_t \mid X_t\right]\right)\right] \mathrm{d}t \\
&\geq \int_0^1 \mathbb{E}\left[c\left(v_t(X_t)\right)\right] \mathrm{d}t \\
&\geq \int_0^1 \mathbb{E}\left[c\left(v_t(Z_t)\right)\right] \mathrm{d}t.
\end{aligned}$$

Key Property: Reflow and Straightening Effect

- The "straightness" (more precisely, geodesicity) of a smooth random process $\boldsymbol{Z} = \{Z_t \colon t \in [0,1]\}$ can be measured by

$$S(\boldsymbol{Z}) = \int_0^1 \mathbb{E}\left\| \dot{Z}_t - (Z_1 - Z_0) \right\|^2 \mathrm{d}t.$$

//Equivalent to the variance of $\dot{Z}_t$ along the trajectory.

$S(\boldsymbol{Z}) = 0 \iff$ Straight trajectories $Z_t = tZ_1 + (1-t)Z_0 \iff$ ODE solved with one Euler step.

Key Property: Straightening

- Following the iterative reflow, we have

$$\{Z_t^{k+1}\} = \texttt{Rectify}(\texttt{Interp}(Z_0^k, Z_1^k)) \quad \Longrightarrow \quad \min_{k \le K} S(\{Z_t^k\}) = \mathcal{O}\left(\frac{1}{K}\right).$$

  - At the fixed point, $S(\boldsymbol{Z}^\infty) = 0$ and the rectified flow is straight.

Key Property: Straightening

- Following the iterative reflow, we have

$$\{Z_t^{k+1}\} = \texttt{Rectify}(\texttt{Interp}(Z_0^k, Z_1^k)) \implies \min_{k \le K} S(\{Z_t^k\}) = \mathcal{O}\left(\frac{1}{K}\right).$$

  - At the fixed point, $S(\boldsymbol{Z}^\infty) = 0$ and the rectified flow is straight.

Proof.

We can show that

$$S(\{Z_t^k\}) \le \mathbb{E}\left[\left\|Z_1^{k-1} - Z_0^{k-1}\right\|^2\right] - \mathbb{E}\left[\left\|Z_1^k - Z_0^k\right\|^2\right]$$

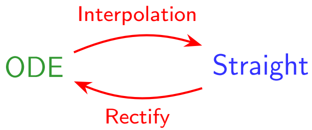
Telescoping summing on $k = 0, \ldots, K$ gives

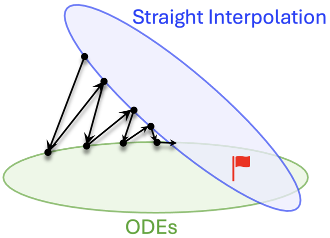
$$\sum_{k=1}^{K} S(Z^k) \le \mathbb{E}\left[\|X_1 - X_0\|^2\right].$$

□

Rectify as Alternative Projection

- Interpolation: enforcing straightness.
- Fitting: enforcing ODE





- In practice, one reflow already very straight transport, as shown in InstaFlow [LZM+23].
- In fact, difficult to find counter examples when reflow is not straight.

Open Question

- When is one reflow sufficient? [Liu22, RBSR24]

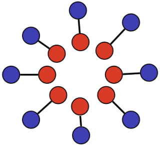
Straight vs. Optimal Transport

Straight Transport = Iterative Rewiring
Optimal Transport = Iterative Rewiring + Derotation.

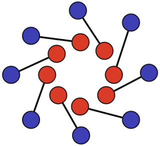
Straight vs. Optimal Couplings

- c-**optimal couplings**: solutions of $\min \mathbb{E}\left[c(Z_1 - Z_0)\right]$.
- **Straight couplings**: the fixed points of the reflow procedure, i.e., $(X_0, X_1) = \texttt{Rectify}((X_0, X_1))$.

- In $\mathbb{R}$, c-optimal couplings = straight couplings = the unique monotonic coupling.
- In $\mathbb{R}^d$ $(d \geq 2)$, c-optimal couplings $\subsetneq$ straight couplings.
- $\texttt{Rectify}(\cdot)$ conducts a kind of multi-objective optimization
  - Tries to decrease the transport for all convex c simultaneously.
  - Can not fully optimize all as different loss functions can be conflicting.



Optimal coupling



Straight, but non-optimal coupling

c-Targeted Rectified Flow

- What if we want to solve the c-optimal transport (OT) problem for a specific c?
  - For example, the standard L2-OT: $c(x) = \|x\|^2$

$$\min_{(X_0, X_1)} \mathbb{E}\left[\|X_1 - X_0\|^2\right], \quad s.t. \quad \mathrm{Law}(X_0) = \pi_0, \ \ \mathrm{Law}(X_1) = \pi_1.$$

- Key: in addition to rewiring trajectories (rectify), we also need to remove the *rotational* component.

Rectified Flow Targeting $c(x) = \frac{1}{2}\|x\|^2$.

Simply restrict the velocity v to be a gradient field ∇f:

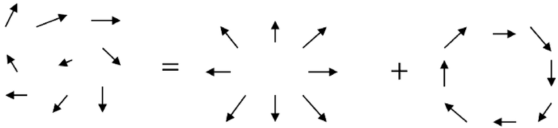
$$\dot{Z}_t = \nabla f(Z_t, t), \qquad Z_0 = X_0,$$

where f is the solution of

$$\min_f \int_0^1 \mathbb{E}\|(X_1 - X_0) - \nabla f(X_t, t)\|^2 \mathrm{d}t.$$

- Yields a **Helmholtz decomposition** on RF velocity v_t:

$$v_t = \nabla f_t + r_t.$$

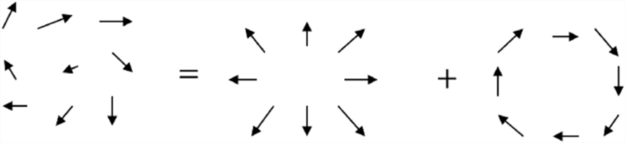


- Related to Knott-Smith and Brenier Theorem, and Benamou-Brenier formula, Hamilton–Jacobi equation, etc

Helmholtz Decomposition

(Weighted) Helmholtz Decomposition: Given a smooth density ρ, any smooth vector field $v\colon \mathbb{R}^d \to \mathbb{R}^d$ admits a decomposition:

$$v(x) = \nabla f(x) + r(x), \quad \text{with} \quad \nabla \cdot (r\rho) = 0.$$



- r is divergence-free (rotational) w.r.t. density ρ.
- The gradient field ∇f captures all divergence (w.r.t. ρ).
- It is an orthogonal decomposition:

$$\mathbb{E}_\rho[\nabla f(x)^\top r(x)] = 0.$$

Proof of Weighted Helmholtz Decomposition.

Problem 1. Approximating v with the best gradient field ∇f:

$$\min_f \mathbb{E}_\rho[\|v(x) - \nabla f(x)\|^2].$$

Problem 2. Approximating v with the best divergence-free field:

$$\min_r \mathbb{E}_\rho[\|v(x) - r(x)\|^2] \quad s.t. \quad \nabla\cdot(r\rho) = 0.$$

These two problems are duality of each other, both equivalent to

$$\max_f \min_r \mathbb{E}\left[\|v(x) - r(x)\|^2 + 2\nabla f(x)^\top r(x)\right].$$

As they are convex optimization, there always exist solutions, which can be shown to coincides with Helmholtz decomposition. □

Removing the rotational components preserves the marginals while decreasing transport cost

Let $\{Z'_t\}$ be the ODE obtained by removing the rotational part from $\{Z_t\}$:

$$\frac{\mathrm{d}}{\mathrm{d}t} Z_t = v_t(Z_t), \qquad \frac{\mathrm{d}}{\mathrm{d}t} Z'_t = \nabla f_t(Z'_t). \quad Z_0 = Z'_0.$$

where v_t yields Helmholtz decomposition:

$$v_t(x) = \nabla f_t(x) + r_t(x), \qquad \text{with} \quad \nabla \cdot (r_t \rho_t) = 0.$$

1) **Marginal preservation**:

$$\mathrm{Law}(Z_t) = \mathrm{Law}(\tilde{Z}_t) \text{ for all time } t.$$

2) **Transport cost reduction**:

$$\int \|\dot{Z}'_t\|^2 \mathrm{d}t \leq \int \|\dot{Z}_t\|^2 \mathrm{d}t.$$

Proof.

1) Marginal preserves as the rotational field does not contribute to the continuity equation:

$$\partial_t \rho_t = -\nabla\cdot(v_t \rho_t) = -\nabla\cdot(\nabla f_t \rho_t) - \underbrace{\nabla\cdot(r_t \rho_t)}_{=0} = -\nabla\cdot(\nabla f_t \rho_t).$$

2) Cost reduces to due to the orthogonality.

$$\begin{aligned}
\int \mathbb{E}\left[\|\dot{Z}_t\|^2\right] \mathrm{d}t &= \int \mathbb{E}\left[\|\nabla f_t(Z_t) + r_t(Z_t)\|^2\right] \mathrm{d}t \\
&= \int \mathbb{E}\left[\|\nabla f_t(Z_t)\|^2 + \|r_t(Z_t)\|^2\right] \mathrm{d}t \quad \text{//orthogonality: } \mathbb{E}\left[\nabla f_t(Z_t)^\top r_t(Z_t)\right] = 0 \\
&\geq \int \mathbb{E}\left[\|r_t(Z_t)\|^2\right] \mathrm{d}t \\
&= \int \mathbb{E}\left[\left\|r_t(Z'_t)\right\|^2\right] \mathrm{d}t \quad \text{//Marginal preservation } \mathrm{Law}(Z_t) = \mathrm{Law}(Z'_t) \\
&= \int \mathbb{E}\left[\|\dot{Z}'_t\|^2\right] \mathrm{d}t.
\end{aligned}$$

□

Rectified Flow Targeting general convex c: $\min \mathbb{E}[c(X_1 - X_0)]$

$$\dot{Z}_t = \nabla c^*(\nabla f(Z_t, t)), \qquad Z_0 = X_0,$$

where v^X minimizes a Fenchel-Young divergence:

$$\min_f \int_0^1 \mathbb{E}\left[c^*(\nabla f(X_t, t)) - (X_1 - X_0)^\top \nabla f(X_t, t) + c(X_1 - X_0)^2\right] \mathrm{d}t.$$

where $c^*(x) := \sup_y \{x^\top y - c(y)\}$ is the convex conjugate of c.

- Related: matching loss, Bregman divergence
- Generalized Helmholtz decomposition: $v_t = \nabla c^*(\nabla f_t) + r_t$
- Only decreases this specific c
- Fixed point $\iff$ c-optimal.
- Reflow can be viewed as a special coordinate descent on dynamic OT