Ph.D. Research Proficiency Examination Presentation

Optimal Mass Transport Theory and Applications

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Outline

Outline

Introduction to Optimal Mass Transport

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Outline

Monge Problem In the 18th cedntury, Monge first introduced a problem minimizing the inter-domain transportation cost while preserving measure quantities, which in modern language is shown as follows:

Problem 1

Given two probability measures $\mu \in \mathbb{P}(X)$ and $\nu \in \mathbb{P}(Y)$, and a cost function $c : X \times Y \to [0, +\infty]$, solve

$$\inf\{M(T) := \int c(x, T(x))d\mu(x) : T_{\#}\mu = \nu\}$$

where we recall that the measure denoted by $T_{\#}\mu$ is defined through $(T_{\#}\mu)(A) := \mu(T^{-1}(A))$ for every A, and is called image measure or fush-forward of μ through T.

The Problem 1 shows that the constraints on T is not closed under weak convergence, this problem is difficult to solve. We will focus on the the generalized problem proposed by Kantorovich[2].

Problem 2

Given $\mu \in \mathbb{P}(X), \nu \in \mathbb{P}(Y)$ and $c : X \times Y \to [0, +\infty]$ we consider the problem

$$\inf\{K(\gamma) := \int_{X\times Y} c d\gamma : \gamma \in \Pi(\mu, \nu)\}$$

where $\Pi(\mu, \nu)$ is the set of the so-called transport plans,

$$\Pi(\mu, \nu) = \{\gamma \in \mathbb{P}(X \times Y) : (\pi_x)_{\#}\gamma = \mu, (\pi_y)_{\#}\gamma = \nu\}$$

where π_x and π_y are the two projections of $X \times Y$ onto X and Y.

The Problem 2 can be rewritten as following:

Problem 3

Given two metric spaces with probabilities measure $(X, \mu), (Y, \nu)$ with the transportation cost function $c : X \times Y \to \mathbb{R}$, the problem is to find the measure preserving map $T : X \to Y$ satisfying condition $\mu(T^{(-1)}(B)) = \nu(B)$, which minimizes the transportation cost $C(T) := \int_X c(x, T(x))d\mu(x)$.

- Intrinsic connection discovered around 1990 by Brenier[3].
- The OMT problem is translated into convex geometry problems.
- Minkowski Problem
- Alexandrov Problem

Problem 4

(**Minkowski problem for compact polytopes in $\mathbb{R}^n$.**) Suppose $n_1, n_2, ..., n_k$ are unit vectors which span $\mathbb{R}^n$ and $A_1, ..., A_k > 0$ so that $\sum_{i=1}^k A_i n_i = 0$. Find a compact convex polytope $P \subset \mathbb{R}^n$ with exactly k codimension-1 faces $F_1, ..., F_k$ so that n_i is the outward normal vector to F_i and the area of F_i is A_i.

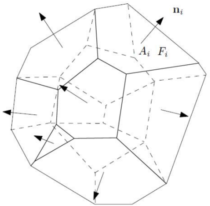

Figure 1: Minkowski problem

Theorem 1

(Alexandrov) Suppose Ω *is a compact convex polytope with non-empty interior in* $\mathbb{R}^n$, $p_1, ..., p_k \subset \mathbb{R}^n$ *are distinct* k *points and* $A_1, ..., A_k > 0$ *so that* $\sum_{i=1}^k A_i = vol(\Omega)$. *Then there exists a vector* $h = (h_1, ..., h_k) \in \mathbb{R}^k$, *unique up to adding the constant*$(c, c, ..., c)$, *so that the piecewise linear convex function*

$$u(x) = \max_{1 \leq i \leq k} \{x \cdot p_i + h_i\}$$

satisfies $vol(\{x \in \Omega | \nabla u(x) = p_i\}) = A_i$

- The graph of the convex function u is an infinite convex polyhedron.
- The PL convex function produces a convex cell decomposition $\{W_i\}$

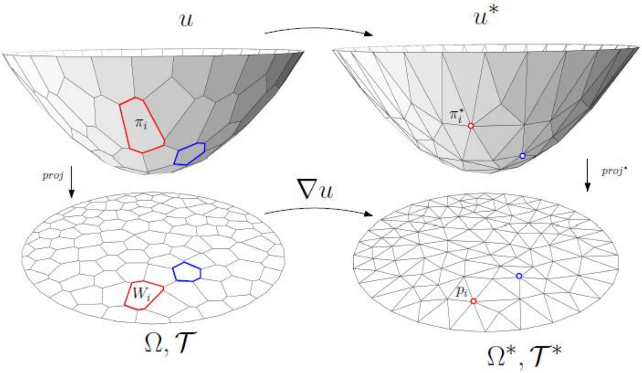

Figure 2: A PL convex function induces a cell decomposition of Ω. Each cell is mapped to a point

Definition 1

(Alexandrov map) The gradient map $\nabla u : x \mapsto \nabla u(x)$ is the Alexandrov map.

- The Alexandrov map is the unique OMT map
- minimizes the energy

$$\int_{\Omega} ||x - T(x)||^2 dx$$

Theorem 2

Let Ω be a compact convex domain in $\mathbb{R}^n$ and $\{p_1, ..., p_k\}$ a set of distinct points in $\mathbb{R}^n$ and $\sigma : \Omega \to \mathbb{R}$ be a positive continuous function. Then for any $A_1, ..., A_k > 0$ with $\sum_{i=1}^k A_i = \int_\Omega \sigma(x)dx$, there exists $b = (b_1, ..., b_k) \in \mathbb{R}^k$, unique up to adding a constant $(c, ..., c)$, so that $\int_{W_i(b)\cap\Omega} \sigma(x)dx = A_i$ for all i. The vectors b are exactly minimum points of the convex function

$$E(h) = \int_a^h \sum_{i=1}^k \int_{W_i(h)\cap\Omega} \sigma(x)dxdh_i - \sum_{i=1}^k h_i A_i$$

on the open convex set $H = \{h \in \mathbb{R}^k | vol(W_i(h) \cap \Omega) > 0 \forall i\}$.

Theorem 2

(continued) In fact, $E(h)$ restricted to $H_0 = H \cap \{h | \sum_{i=1}^k h_i = 0\}$ is strictly convex. Furthermore, ∇u_b minimizes the quadratic cost $\int_\Omega |x - T(x)|^2 \sigma dx$ among all transport maps $T : (\Omega, \sigma dx) \to (\mathbb{R}^n, \sum_{i=1}^k A_i \delta_{p_i})$. where u_b is defined as the PL convex function

$$u_b(x) = \max_i \{x \cdot p_i + b_i\}$$

and the closed convex polytope is denoted as

$$W_i(h) = \{x \in \mathbb{R}^n | \nabla u(x) = p_i\} = \{x | x \cdot p_i + b_i \geq x \cdot p_j + b_j \textit{ for all } j\}$$

- Voronoi Diagram $\forall\ p$, the convex region $R(p) = \{x \in E^d | d(x,p) < d(x,q), \forall q \in M - \{p\}\}$.
- Power Voronoi Diagram Use power distance as follows instead of standard L^2 distance metric.

$$POW(x, p_i) = \frac{1}{2}||x - p_i||^2 - \frac{1}{2}h_i.$$

- Power Diagram is a partition of Euclidean plane into polygonal cells,

$$W_i = \{x | Pow(x, p_i) \leq Pow(x, p_j), \forall j\}.$$

- Computing the Power Diagram is equivalent to computing the Alexandrov map.

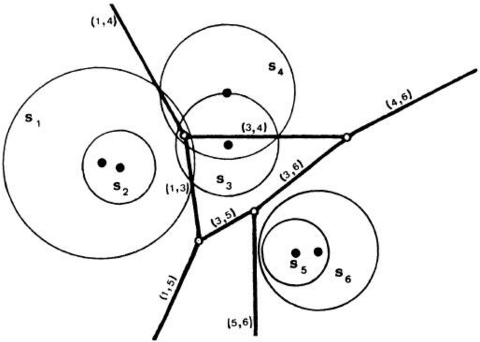

Figure 3: Power diagram for 6 circles. A partition of the Euclidean plane.

The following theorem presents the link of Optimal mass transport and the Monge-Ampere Equation[4]:

Theorem 3

Let μ and ν be two compactly supported probability measures on $\mathbb{R}^n$. If μ is absolutely continuous with respect to the Lebesgue measure, then

i. *there exists a unique solution T to the optimal transport problem with cost $c(x, y) = |x - y|^2/2$;*
ii. *there exists a convex function $u : \mathbb{R}^n \to \mathbb{R}$ such that the optimal map T is given by $T(x) = \nabla u(x)$ for $\mu - a.e.\ x$*

Theorem 3

(continued) Furthermore, if $\mu(dx) = f(x)dx$ and $\nu(dy) = g(y)dy$, then T is differentiable $\mu - a.e.$ and

$$|det(\nabla T(X))| = \frac{f(x)}{g(T(x))} \quad for\ \mu - a.e.\ x \in \mathbb{R}^n.$$

Since $T = \nabla u$,[3], the formula becomes:

$$det(D^2 u(x)) = \frac{f(x)}{g(\nabla(u))}$$

which is a non-linear elliptic PDE.

Definition 2

(Shape Distance). Given two Riemannian surfaces, which are topological disks, $(S_1, \mathbf{g}_1)$ and $(S_2, \mathbf{g}_2)$, the Riemann mappings are ϕ_k, $k = 1, 2$ respectively. Let $\eta \in Mob(\mathbb{D})$ be a Mobius transformation, where $Mob(\mathbb{D})$ is the Mobius transformation group of the unit planar disk, then $\eta_k \circ \phi_k$ are still Riemann mappings. Each Riemann mapping $\eta_k \circ \phi_k$ determines a unique optimal transportation map $\tau_k(\phi_k, \eta_k)$. Then the distance between two surfaces is given by

$$d(S_1, S_2) := \min_{\eta_1, \eta_2 \in Mob(\mathbb{D})} \int_{\mathbb{D}} |\tau_1(\phi_1, \eta_1) - \tau_2(\phi_2, \eta_2)|^2 dxdy$$

$(M, \mathbf{g})$ is a Riemannian manifold with a Riemannian metric $\mathbf{g}$, consider the set:

$$P_p(M) := \{\mu \in P(M) : \int |x|^p d\mu < +\infty\}.$$

For $\mu, \nu \in P_p(M)$, we will define

$$W_p(\mu, \nu) := \inf_{T_{\#}\mu=\nu} (\int_M d(x, T(x))^p d\mu(x))^{\frac{1}{p}}.$$

Then, The quantity W_p defined above is a distance over $P_p(M)$

- $W_p(\mu, \nu) \geq 0$.
- $W_p(\mu, \nu) = 0$ implies $\mu = \nu$.
- Satisfies triangle inequality.

Definition 3

Given a Polish space X, for each $p \in [1, +\infty)$, the Wasserstein space of order p, $\mathbb{W}_p(X)$, is defined as the space $P_p(X)$ endowed with the distance W_p.

Outline

Surfaces are usually represented as *Triangular Mesh* in discrete settings.

- Faces, edges, vertices.
- Discrete Riemannian Metric
- Discrete Gauss Curvature
- Delaunay Triangulation

Definition 4

(Discrete Riemannian Metric). A discrete metric on a triangular mesh (S, T) is a function defined on the edges $d : E \to \mathbb{R}^+$, which satisfies the triangle inequality, on a face $[v_i, v_j, v_k]$,

$$d_{ij} + d_{jk} > d_{ki}; d_{ki} + d_{ij} > d_{jk}; d_{ik} + d_{kj} > d_{ji}.$$

Definition 5

(Delaunay Triangulation). Aclosed discrete surface (S, T) with a discrete metric d, we say a triangulation T is Delaunay, if for any edge $[v_i, v_j]$ adjacent to two faces $[v_i, v_j, v_k]$ and $[v_j, v_i, v_l]$,

$$\theta_k^{ij} + \theta_l^{ji} \leq \pi,$$

where θ_k^{ij} is the corner angle at v_k in $[v_i, v_j, v_k]$, and θ_l^{ji} is the angle at v_l in $[v_j, v_i, v_l]$.

Definition 6

(Discrete Gauss Curvature). The discrete Gauss curvature function on a mesh is defined on vertices, $K : V \to \mathbb{R}$, such that

$$K(v) = \begin{cases} 2\pi - \sum_i \theta_i, & v \notin \partial S \\ \pi - \sum_i \theta_i, & v \in \partial S \end{cases}$$

where θ_i's are corner angles adjacent to the vertex v, and ∂S represents the boundary of the mesh.
Gauss-Bonnet:

$$\sum_i K(v_i) = 2\pi\chi(S)$$

where $\chi(S)$ is the Euler characteristic of S.

Definition 7

(Discrete Yamabe Flow). Given a surface (S, V) with a discrete metric d, given a target curvature function $\bar{K} : V \to \mathbb{R}$, $\bar{K}(v_i) \in (-\infty, 2\pi)$, and the total target curvature satisfies Gauss-Bonnet formula, the discrete Yamabe flow is defined as

$$\frac{du(v_i)}{dt} = \bar{K}(v_i) - K(v_i),$$

under the constraint $\sum_{v_i \in V} u(v_i) = 0$. During the flow, the triangulation on (S, V) is updated to be Delaunay with respect to $d(t)$, for all time t.

The existence of the solution to the Yamabe flow is guarranteed by the following theorem.

Theorem 4

Suppose (S, V) *is a closed connected surface and* d *is any discrete metric on* (S, V). *Then for any* $\bar{K} : V \to (-\infty, 2\pi)$ *satisfying Gauss-Bonnet formula, there exists a discrete metric* $\bar{d}$, *unique up to a scaling on* (S, V), *so that* $\bar{d}$ *is discrete conformal to* d *and the discrete curvature of* $\bar{d}$ *is* $\bar{K}$. *Furthermore, the* $\bar{d}$ *can be obtained by discrete Yamabe flow.*

Algorithms

Algorithm 1 Discrete Surface Yamabe Flow

Require: The inputs include: a triangular mesh Σ, A target curvature $\bar{K}$
Ensure: : A discrete metric

```
Initialize the discrete conformal factor u as 0 and conformal structure
coefficient η, such that η(e) equals to the initial edge length of e.
while max_i |K̄_i − K_i| > ϵ do
    compute the edge length from γ and η
    Update the triangulation to be Delaunay using diagonal edge swap
    for each pair of adjacent faces
    Compute the corner angle θ_i^{jk} from the edge length using cosine law
    Compute the vertex curvature K
    Compute the Hessian matrix H
    Solve linear system Hδu = K̄ − K
    Update conformal factor u ← u − δu
end while
Output the result metric
```

The Hessian matrix H is defined explicitly:

$$h_{ij} = \begin{cases} -w_{ij} & v_i \sim v_j \ i \neq j \\ 0 & v_i \nsim v_j \ i \neq j \\ \sum_k w_{ik} & i = j \end{cases}$$

where w_{ij} is the cotangent edge weight defined as

$$w_{ij} := \begin{cases} cot\theta_k^{ij} + cot\theta_l^{ji} & [v_i, v_j] \notin \partial S \\ cot\theta_k^{ij} & [v_i, v_j] \in \partial S \end{cases}$$

Outline

Theorem 5

For any given measure ν, such that

$$\sum_{j=1}^{n} \nu_j = \int_{\Omega} \mu, \nu_j > 0,$$

there must exist a height vector $\mathbf{h}$ *unique up to adding a constant vector* $(c, c, ..., c)$*, the convex function* $u_{\mathbf{h}}(x)$ *induces the cell decomposition of* $\Omega = \cup_{i=1}^{k} W_i(\mathbf{h})$*, such that the folloing area-preserving constraints are satisfied for all cells,*

$$\int_{W_i(\mathbf{h})} = \nu_i, \ \ i = 1, 2, ..., n.$$

Theorem 5

Furthermore, the gradient map *grad* $u_{\mathbf{h}}$ optimizes the transportation cost

$$C(T) := \sum_{\Omega} |x - T(x)|^2 \mu(x) dx.$$

Theorem 6

Let Ω be a compact convex domain in $\mathbb{R}^n$, $\{p_1, ..., p_k\}$ be a set of distinct points in $\mathbb{R}^n$ and $\sigma : \Omega \to \mathbb{R}$ be a positive continuous function. Then for any $A_1, ..., A_k > 0$ with $\sum_{i=1}^k A_i = \int_\Omega \sigma(x)dx$, there exists $b = (b_1, ..., b_k) \in \mathbb{R}^k$, unique up to adding a constant $(c, c, ..., c)$, sothat $\int_{W_i(b)\cap\Omega} sigma(x)dx = A_i$ for all i. The vectors b are exactly minimum points of the convex function

$$E(h) = \int_a^h \sum_{i=1}^k \int_{W_i(h)\cap\Omega} \sigma(x)dxdh_i - \sum_{i=1}^k h_i A_i$$

on the open convex set $H = \{h \in \mathbb{R}^k | vol(W_(h) \cap \Omega) > 0 \text{ for all } i\}$. Furthermore, ∇u_b minimizes the quadratic cost $\int_\Omega |x - T(x)|^2 \sigma(x)dx$ among all transport maps $T : (\Omega, \sigma dx) \to (\mathbb{R}^n, \sum_{i=1}^k A_i \delta_{p_i})$

In practice, the energy can be optimized using Newton's method, with the help of the computation of the energy gradient

$$\nabla E(\mathbf{h}) = (w_1(\mathbf{h}) - \nu_1), \ldots, w_k(\mathbf{h}) - \nu_k)^T$$

. The Hessian of $E(\mathbf{h})$ is given as following:

$$\frac{\partial^2 E(\mathbf{h})}{\partial h_i \partial h_j} = \begin{cases} \frac{\int_{e_{ij}} \mu(x)dx}{|y_j - y_i|} & W_i(\mathbf{h}) \cap W_j(\mathbf{h}) \cap \Omega \neq \emptyset \\ 0 & otherwise \end{cases}$$

Algorithm 2 Optimal Mass Transport Map

Require: The Input: (Ω,μ),(P,ν), $\nu_i > 0$, $\int_\Omega u(x)dx = \sum_{i=1}^k \nu_i$

The Output: The unique discrete OMT-Map $f : (\Omega,\mu) \to (P,\nu)$

```
Scale and translate P, such that P ⊂ Ω
h ← (0, 0, ..., 0)
Compute the power diagram D(h),dual power Delaunay triangulation
    T(h),the cell areas w(h) = (w_1(h), ..., w_k(h))
while ||∇E|| < ε do
    Compute ∇E and Hessian matrix
    λ ← 1
    h ← h − λH^{-1}∇E(h)
    Compute D(h), T(h), and w(h)
    while ∃w_i(h) == 0 do
        Update h ← h + λH^{-1}∇E(h), λ ← (1/2)λ,h ← h − λH^{-1}∇E(h)
        Compute D(h), T(h), and w(h)
    end while
end while
Output the result mapping f : Ω → P, W_i(h) → p_i, i = 1, 2, ..., k.
```

Outline

Suppose S is a topological disk, with Riemannian metric g. Scale the surface so that the area is π. According to Riemann Mapping theorem, there is a conformal mapping $\phi : (S, \mathbf{g}) \to (\mathbb{D}, dzd\bar{z})$, such that $\mathbf{g} = e^{2\lambda(z)}dzd\bar{z}$. Then we can find the OMT map $\tau : (\mathbb{D}, dzd\bar{z}) \to (\mathbb{D}, e^{2\lambda}dzd\bar{z})$, and the composition $\tau^{-1} \circ \phi : (S, \mathbf{g}) \to (\mathbb{D}, dzd\bar{z})$ gives the area-preserving mapping.

Algorithm 3 Topological Disk Area-preserving Parameterization

Require: The inputs: a triangular mesh M, which is a topological disk; three vertices $\{v_0, v_1, v_2\} \subset \partial M$
The output: The area-preserving parameterization $f : M \to \mathbb{D}$, which maps $\{v_0, v_1, v_2\}$ to $\{1, i, -1\}$ respectively.

1: Scale M such that the total area is π
2: Compute the conformal parameterization $\phi : M \to \mathbb{D}$, such that the images of $\{v_0, v_1, v_2\}$ are $\{1, i, -1\}$
3: For each vertex $v_i \in M$, define $p_i = \phi(v_i)$, ν_i to be $\frac{1}{3}$ of the total area of the faces adjacent to v_i. Set $P = \{p_i\}, \nu = \{\nu_i\}$
4: Compute the *Discrete Optimal Mass Transport Map* with Algorithm 2
5: Construct the mapping $\tau^{-1} \circ \phi : M \to \mathbb{D}$, which maps each vertex $v_i \in M$ to the centroid of $W_i(\mathbf{h}) \subset \mathbb{D}$

Outline

Theorem 7

(Polar Factorization[3]). Let Ω_0 *and* Ω_1 *be two convex subdomains of* $\mathbb{R}^n$ *with smooth boundaries, each with a positive density function* μ_0, μ_1 *respectively, and of the same total mass* $\int_{\Omega_0} \mu_0 = \int_{\Omega_1} \mu_1$*. Let* $\phi : (\Omega_0, \mu_0) \to (\Omega_1, \mu_1)$ *be an diffeomorphic mapping, then* ϕ *has a unique decomposition of the form*

$$\phi = (\nabla u) \circ s$$

where $u : \Omega_0 \to \mathbb{R}$ *is a convex function,* $s : (\Omega_0, \mu_0) \to (\Omega_0, \mu_0)$ *is a measure-preserving mapping. This is called a polar factorization of* ϕ *with respect to* μ_0*.*

A diffeomorphism $\phi : (\Omega_0, \mu_0) \to (\Omega_1, \mu_1)$, where $\mu_1 = \phi_{\#}\mu_0$, can be decomposed to the composition of a measure preserving map $s : (\Omega_0, \mu_0) \to (\Omega_0, \mu_0)$ and a L^2 optimal mass transportation map [3] $\nabla u : (\Omega_0, \mu_0) \to (\Omega_1, \mu_1)$, and the composition is unique.
According to *Polar Decomposition*, $\nabla u^* = (\nabla u)^{-1} : (\Omega_1, \mu_1) \to (\Omega_0, \mu_0)$ is also an optimal transportation map. The measure-preserving map s can be computed directly by $s = (\nabla u)^{-1} \circ \phi$.

Algorithm 4 Polar Factorization of Mapping

Require: Convex domains Ω_0 and Ω_1 in $\mathbb{R}^d$. A diffeomorphic mapping $\phi : (\Omega_0, \mu_0) \to (\Omega_1, \mu_1)$, satisfying $\mu_1 = \phi_{\#}\mu_0$.

Ensure: The polar factorization $\phi = \nabla u \circ s$, where s is measure-preserving and u is convex.

Compute the unique optimal mass transportation map $\nabla v : (\Omega_1, \mu_1) \to (\Omega_0, \mu_0)$ using Alg.2. The convex function u is the Legendre dual of v, $u = v^*$

Compute the composition $s = \nabla v \circ \phi$

The conformal mapping of a Sphere surface, approximated by a triangle mesh, is obtained by two steps.

- Conformally mapped to a unit sphere using spherical harmonic mapping
- Conformally mapped onto the complex plane using the stereo-graphic projection.

Sharp Distinction: unbounded cells with finite areas under the spherical measure.

For a finite polygon G,

$$Area(G) = -\sum_i \int_{s_i} k_g ds.$$

For a infinite polygon G, take the exterior angle at ∞ to be $\pi - \theta$, and use Gauss-Bonnet Theorem to get a similar formula.

Outline

After we have the OMT map between two surfaces M_1, M_2 with topological disk algorithm, we will have the map: $f : \Omega \to P, W_i(\mathbf{h}) \to p_i$. Therefore, the Wasserstein distance between M_1 and M_2 can be defined as

$$d_W(\mu,\nu) = \sum_{i=1}^{n} \int_{W_i} (x - p_i)^2 \mu(x) dx$$

Algorithm 5 Computing Wasserstein Distance for Two Surfaces

Require: The Inputs: Two topological disk surfaces: $(M_1, g_1), (M_2, g_2)$.
The Outputs: The Wasserstein distance between M_1 and M_2

1: Scale and normalize M_1 and M_2 such that the total area of each is π.
2: Compute the conformal maps $\phi_1 : M_1 \to \mathbb{D}_1$, and $\phi_2 : M_2 \to \mathbb{D}_2$ defined above.
3: Construct the convex planar domain (Ω, μ) from $\mathbb{D}_1$
4: Discretize $\mathbb{D}_2$ into a planar point set with measure (P, ν)
5: With (Ω, μ) and (P, ν) as inputs, compute the Optimal Mass Transport map f with Algorithm 2
6: Output the Wasserstein distance $d_W(\mu, \nu)$.

Second Slide Title

- First item.

Second Slide Title

- First item.
- Second item.

Second Slide Title

- First item.
- Second item.
- Third item.

Second Slide Title

- First item.
- Second item.
- Third item.
- Fourth item.

Second Slide Title

- First item.
- Second item.
- Third item.
- Fourth item.
- Fifth item.

Second Slide Title

- First item.
- Second item.
- Third item.
- Fourth item.
- Fifth item. Extra text in the fifth item.

Outline

Blocks

Block Title

You can also highlight sections of your presentation in a block, with it's own title

Theorem 8

There are separate environments for theorems, examples, definitions and proofs.

Example 9

Here is an example of an example block.

Summary

- The first main message of your talk in one or two lines.
- The second main message of your talk in one or two lines.
- Perhaps a third message, but not more than that.

- Outlook
  - Something you haven't solved.
  - Something else you haven't solved.

For Further Reading I

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