$$\nabla f + \sum_k \lambda_k \nabla g_k$$

Optimization Techniques

for Geometry Processing

Justin Solomon
MIT

David Bommes
RWTH Aachen University

$$\nabla f + \sum_k \lambda_k \nabla g_k$$

(Variational)

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Optimization Techniques for Geometry Processing

Swiss Army Knife

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More Specifically

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \ & f(x) \\ \text{s.t.} \ & g(x) = 0 \\ & h(x) \geq 0 \end{aligned}$$

Two Roles

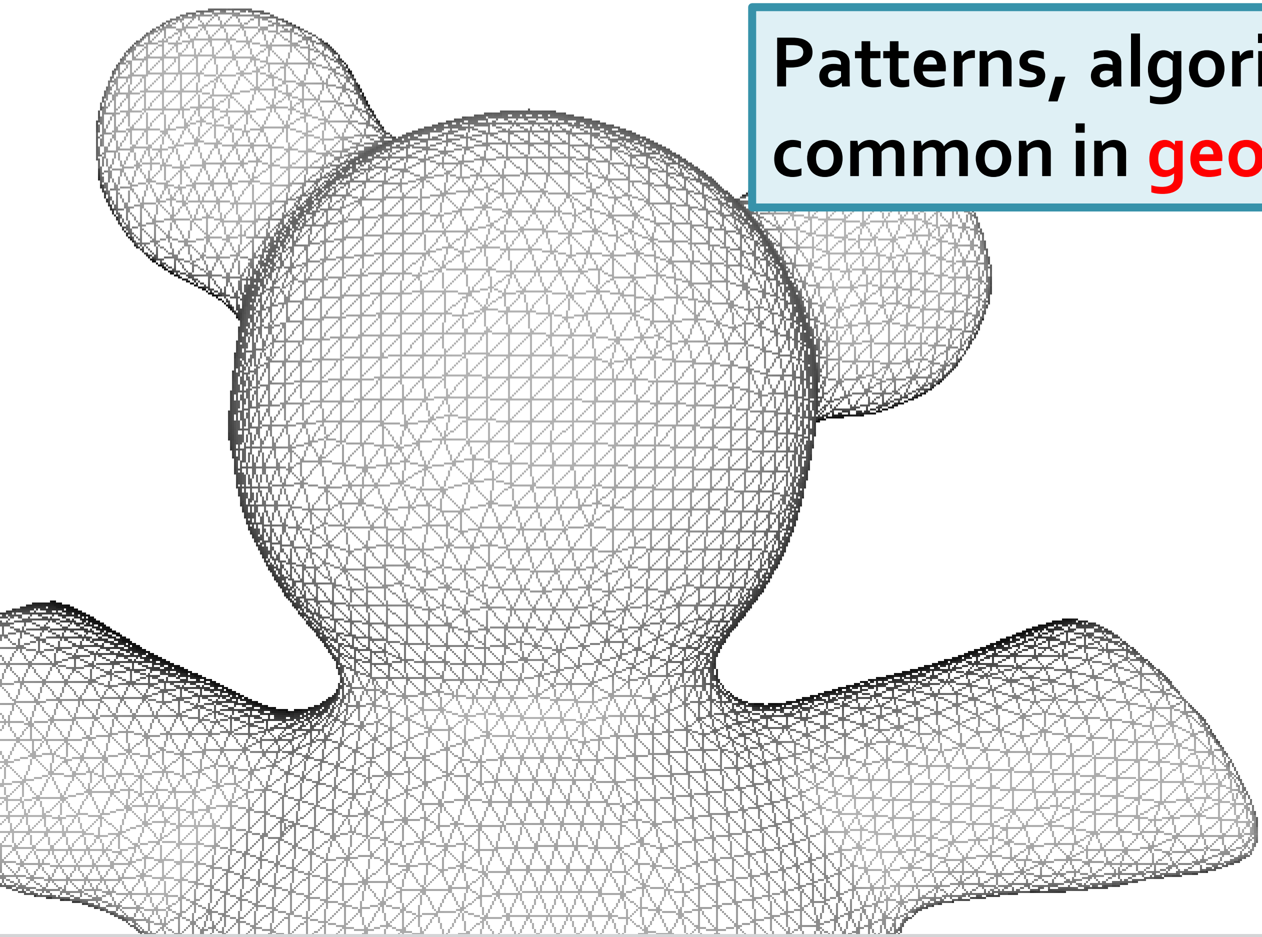
- **Client**

  Which optimization tool is relevant?

- **Designer**

  Can I design an algorithm for this problem?

Our Bias



Patterns, algorithms, & examples common in **geometry processing**.

Optimization is a <u>huge</u> field.

Rough Plan

Part I (Justin)

- Vocabulary
- Simple examples
- Unconstrained optimization
- Equality-constrained optimization

Rough Plan

Part II (David)

- Inequality constraints
- Advanced algorithms
- Discrete problems
- Conclusion

Rough Plan

Part I (Justin)

- **Vocabulary** (basic material!)
- Simple examples
- Unconstrained optimization
- Equality-constrained optimization

Optimization Terminology

$$\min_{x \in \mathbb{R}^n} \boxed{f(x)}$$
$$\text{s.t. } g(x) = 0$$
$$h(x) \geq 0$$

Objective ("Energy Function")

Optimization Terminology

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \ & f(x) \\ \text{s.t.} \ & g(x) = 0 \\ & h(x) \geq 0 \end{aligned}$$

Equality Constraints

Optimization Terminology

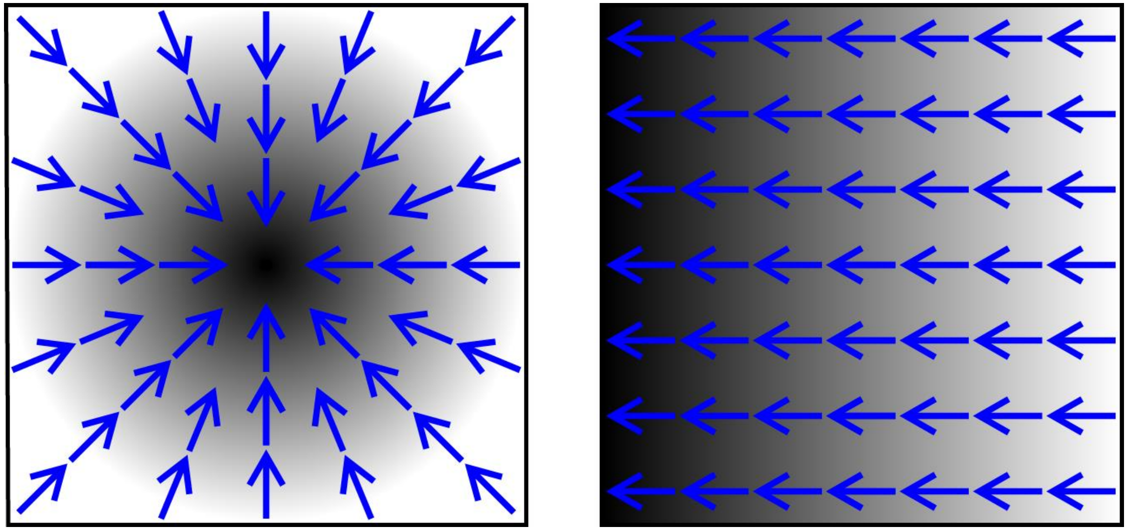
$$\min_{x\in\mathbb{R}^n} f(x)$$
$$\text{s.t. } g(x) = 0$$
$$h(x) \geq 0$$

Inequality Constraints

Optimization Terminology

$$f : \mathbb{R}^n \to \mathbb{R}$$

$$\to \nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n} \right)$$



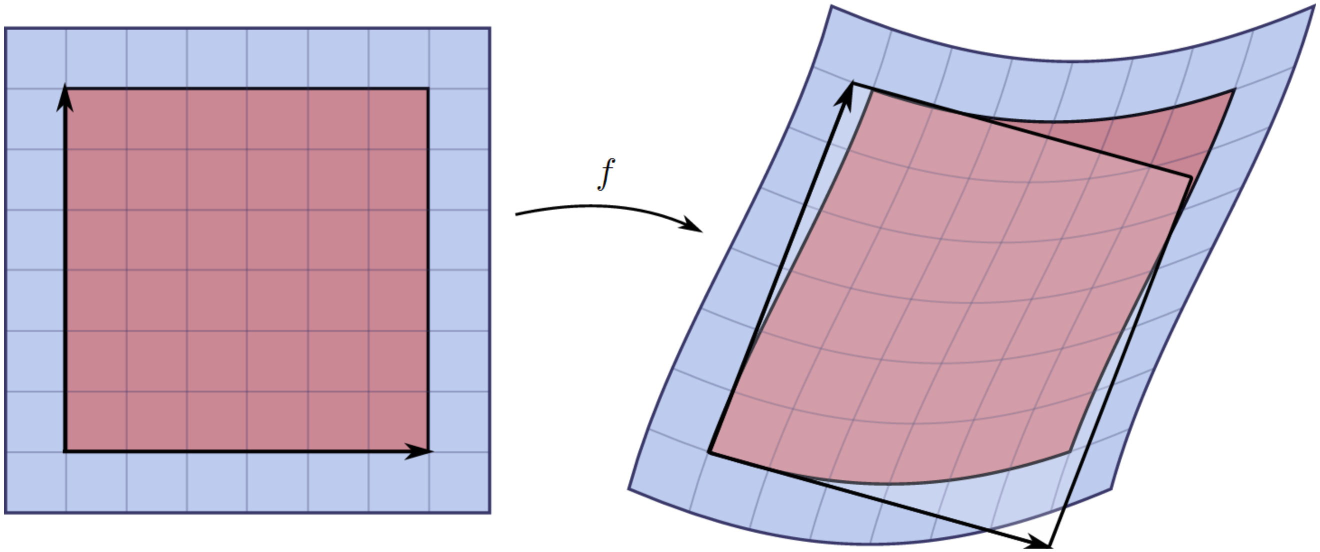
https://en.wikipedia.org/?title=Gradient

Gradient

Optimization Terminology

$$f : \mathbb{R}^n \to \mathbb{R}^m$$

$$\to (Df)_{ij} = \frac{\partial f_i}{\partial x_j}$$

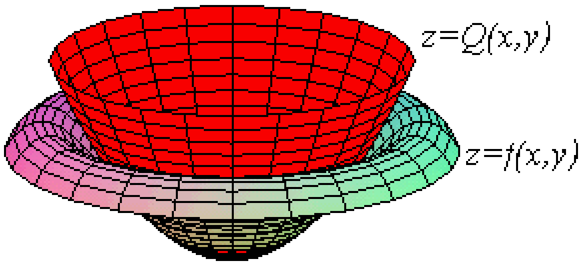


https://en.wikipedia.org/wiki/Jacobian_matrix_and_determinant

Jacobian

Optimization Terminology

$$f:\mathbb{R}^n \to \mathbb{R} \to H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$



$$f(x) \approx f(x_0) + \nabla f(x_0)^\top (x - x_0) + (x - x_0)^\top Hf(x_0)(x - x_0)$$

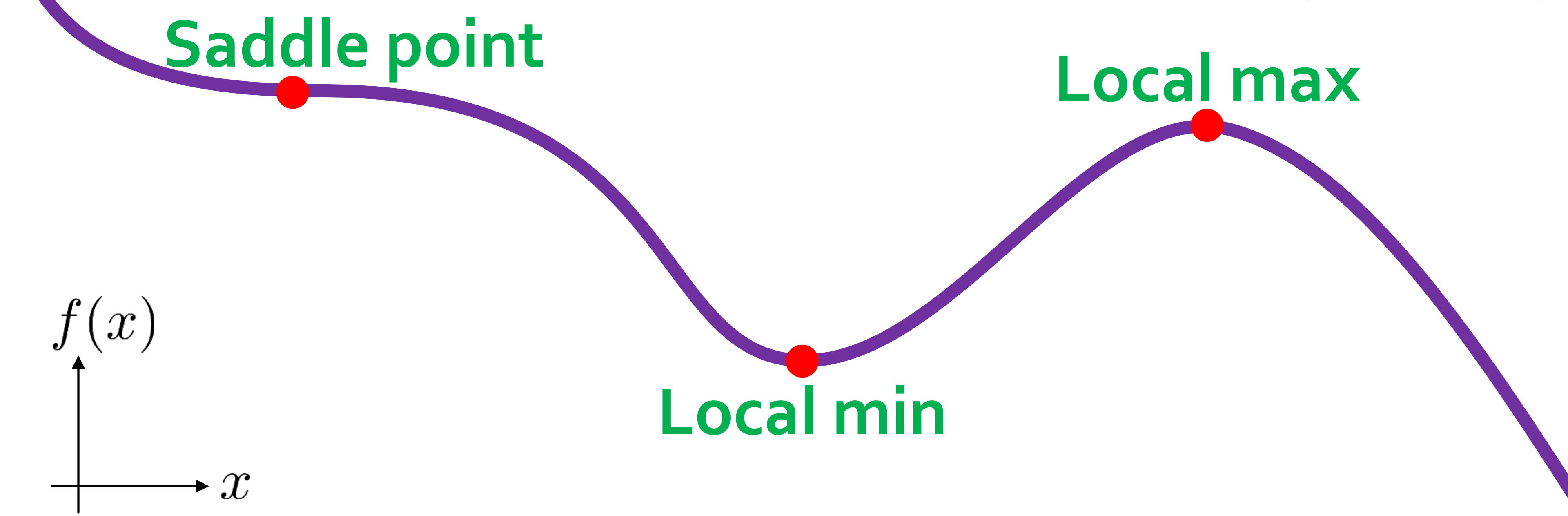
http://math.etsu.edu/multicalc/prealpha/Chap2/Chap2-5/10-3a-t3.gif

Hessian

Optimization Terminology

$$\nabla f(x) = 0$$

(unconstrained)



Critical point

Rough Plan

Part I (Justin)

- Vocabulary
- **Simple examples**
- Unconstrained optimization
- Equality-constrained optimization

Encapsulates Many Problems

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \; & f(x) \\ \text{s.t.}\; & g(x) = 0 \\ & h(x) \geq 0 \end{aligned}$$

$$Ax = b \leftrightarrow f(x) = \|Ax - b\|_2$$

$$Ax = \lambda x \leftrightarrow f(x) = \|Ax\|_2, g(x) = \|x\|_2 - 1$$

$$\text{Roots of } g(x) \leftrightarrow f(x) = 0$$

Q:

How effective are generic optimization tools?

Q:

How effective are **generic** optimization tools?

Not very!

Generic Advice

Try the

simplest solver first.

Quadratic with Linear Equality

$$\begin{array}{ll} \min_x & \frac{1}{2}x^\top A x - b^\top x + c \\ \text{s.t.} & Mx = v \end{array}$$

(assume A is symmetric and positive definite)

$$\left(\begin{array}{cc} A & M^\top \\ M & 0 \end{array}\right)\left(\begin{array}{c} x \\ \lambda \end{array}\right) = \left(\begin{array}{c} b \\ v \end{array}\right)$$

Special Case: Least-Squares

$$\min_x \frac{1}{2}\|Ax - b\|_2^2$$

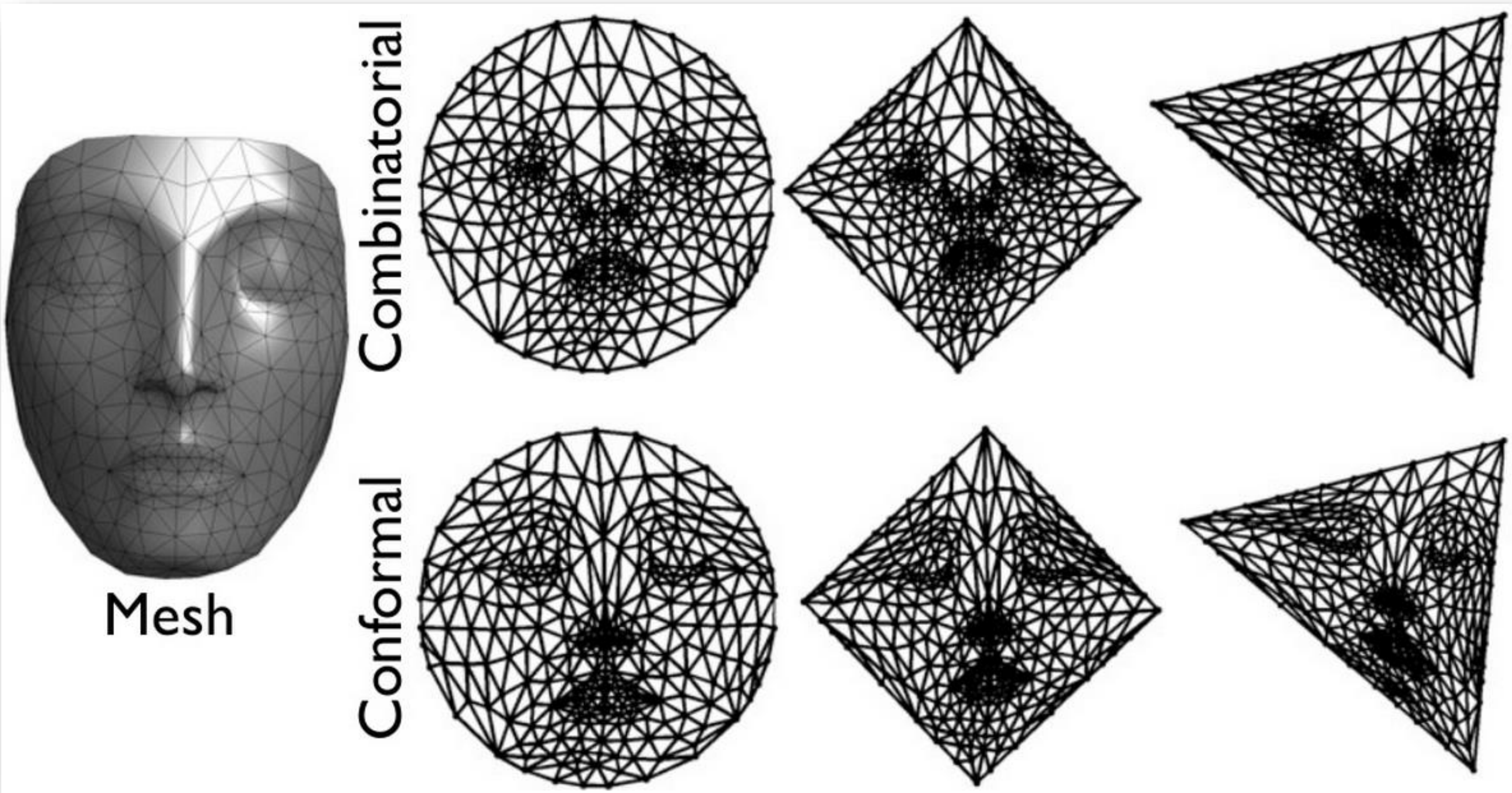
$$\to \min_x \frac{1}{2} x^\top A^\top A x - b^\top A x + \|b\|_2^2$$

$$\implies A^\top A x = A^\top b$$

Normal equations

(better solvers for this case!)

Example: Mesh Embedding



G. Peyré, mesh processing course slides

Linear Solve for Embedding

$$\begin{aligned} \min_{x_1,\ldots,x_{|V|}} \quad & \sum_{(i,j)\in E} w_{ij} \|x_i - x_j\|_2^2 \\ \text{s.t.} \quad & x_v \text{ fixed } \forall v \in V_0 \end{aligned}$$

- **$w_{ij} \equiv 1$:** Tutte embedding
- **w_{ij} from mesh:** Harmonic embedding

Assumption: w symmetric.

More tomorrow!

Linear Solver Considerations

- **Never construct A^{-1} explicitly**
  (if you can avoid it)

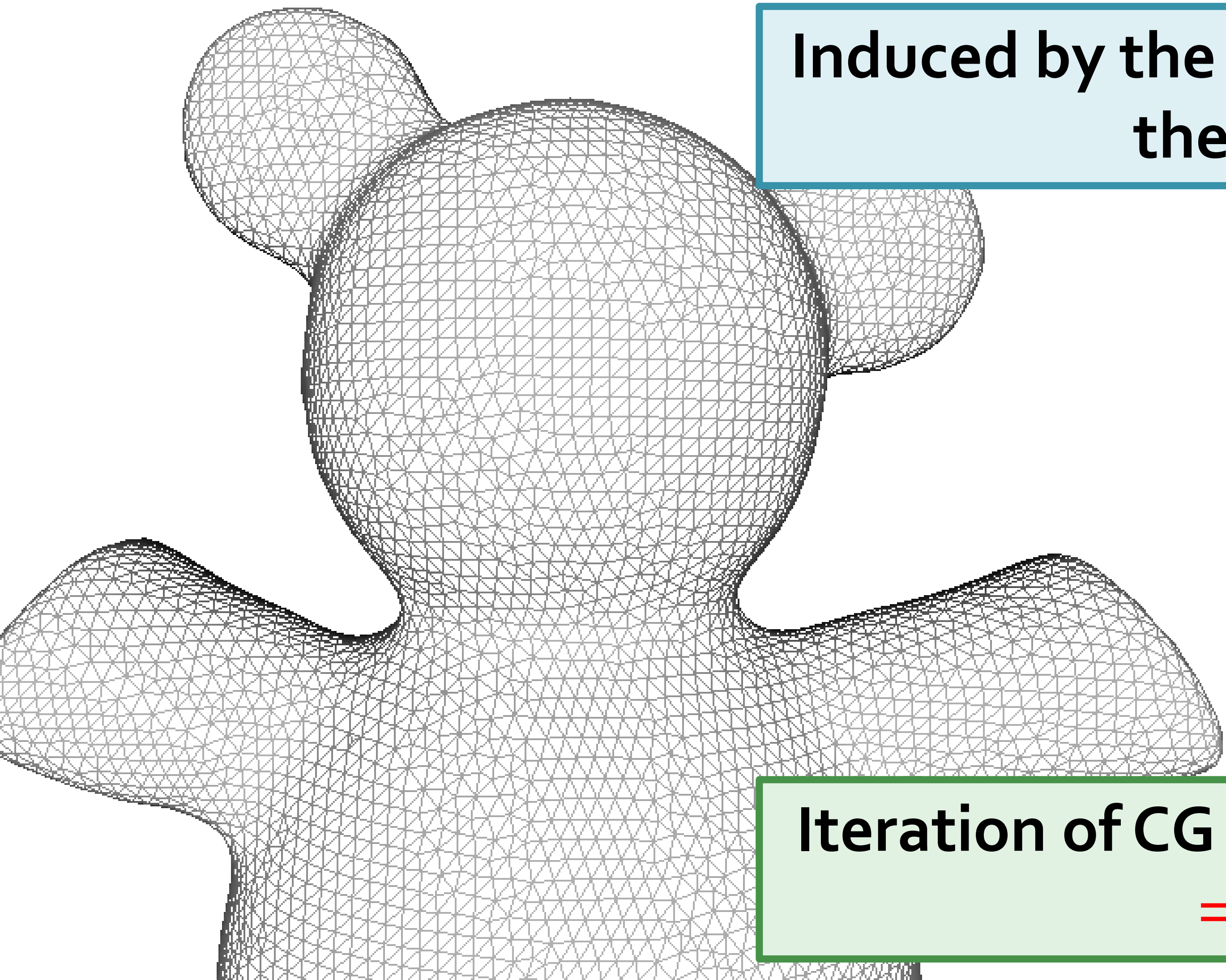
- **Added structure helps**
  <u>Sparsity</u>, symmetry, positive definiteness

$$\texttt{inv(A)*b} \ll \texttt{(A'*A)\textbackslash(A'*b)} \ll \texttt{A\textbackslash b}$$

Two Classes of Solvers

- **Direct** (***explicit*** **matrix)**
  - Dense: Gaussian elimination/LU, QR for least-squares
  - Sparse: Reordering (SuiteSparse, Eigen)
- **Iterative** (***apply*** **matrix repeatedly)**
  - Positive definite: Conjugate gradients
  - Symmetric: MINRES, GMRES
  - Generic: LSQR

Very Common: Sparsity



Induced by the **connectivity** of the triangle mesh.

Iteration of CG has local effect
⇒ **Precondition!**

Returning to Parameterization

$$\begin{aligned} \min_{x_1,\ldots,x_{|V|}} \quad & \sum_{(i,j)\in E} w_{ij} \|x_i - x_j\|_2^2 \\ \text{s.t.} \quad & x_v \text{ fixed } \forall v \in V_0 \end{aligned}$$

What if $V_0 = \{\}$?

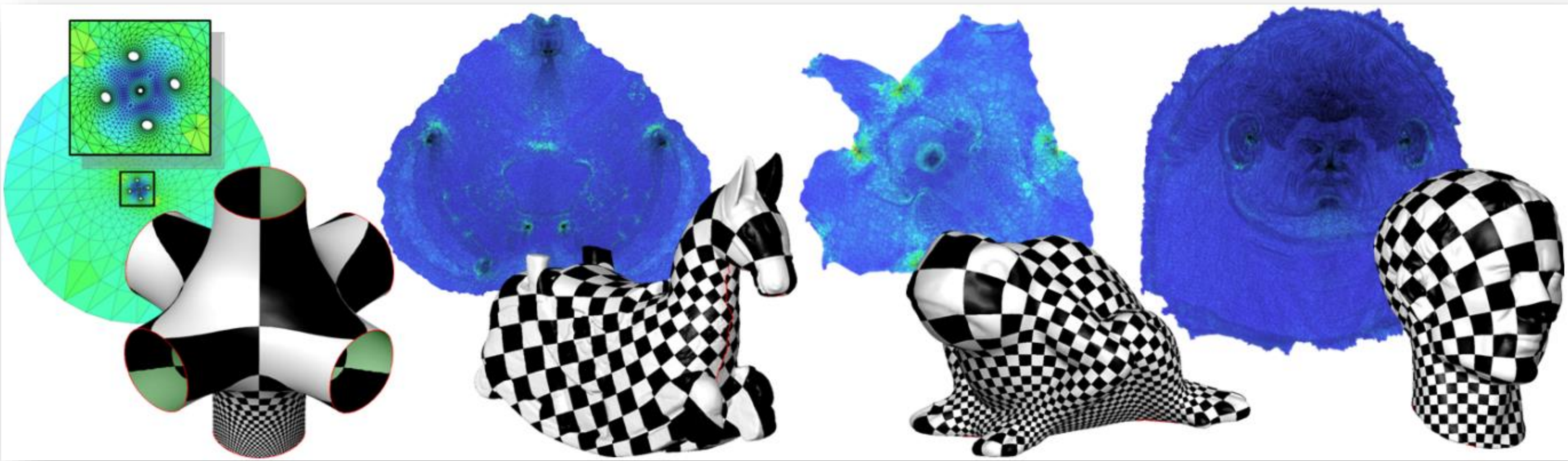
Nontriviality Constraint

$$\left\{ \begin{array}{rl} \min_x & \|Ax\|_2 \\ \text{s.t.} & \|x\|_2 = 1 \end{array} \right\} \mapsto A^\top A x = \lambda x$$

Prevents trivial solution $x \equiv 0$.

Extract the smallest eigenvalue.

Back to Parameterization



Mullen et al. "Spectral Conformal Parameterization." SGP 2008.

$$\min_{\substack{u \\ u^\top Be=0 \\ u^\top Bu=1}} \quad u^\top L_C u \quad \longleftrightarrow \quad L_c u = \lambda B u$$

$u^\top Be=0$ ← *Easy fix*

Basic Idea of Eigenalgorithms

$$
\begin{aligned}
A\vec{v} &= c_1 A\vec{x}_1 + \cdots + c_n A\vec{x}_n \\
&= c_1 \lambda_1 \vec{x}_1 + \cdots + c_n \lambda_n \vec{x}_n \text{ since } A\vec{x}_i = \lambda_i \vec{x}_i \\
&= \lambda_1 \left(c_1 \vec{x}_1 + \frac{\lambda_2}{\lambda_1} c_2 \vec{x}_2 + \cdots + \frac{\lambda_n}{\lambda_1} c_n \vec{x}_n \right) \\
A^2\vec{v} &= \lambda_1^2 \left(c_1 \vec{x}_1 + \left(\frac{\lambda_2}{\lambda_1}\right)^2 c_2 \vec{x}_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^2 c_n \vec{x}_n \right) \\
&\vdots \\
A^k\vec{v} &= \lambda_1^k \left(c_1 \vec{x}_1 + \left(\frac{\lambda_2}{\lambda_1}\right)^k c_2 \vec{x}_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^k c_n \vec{x}_n \right).
\end{aligned}
$$

Combining Tools So Far

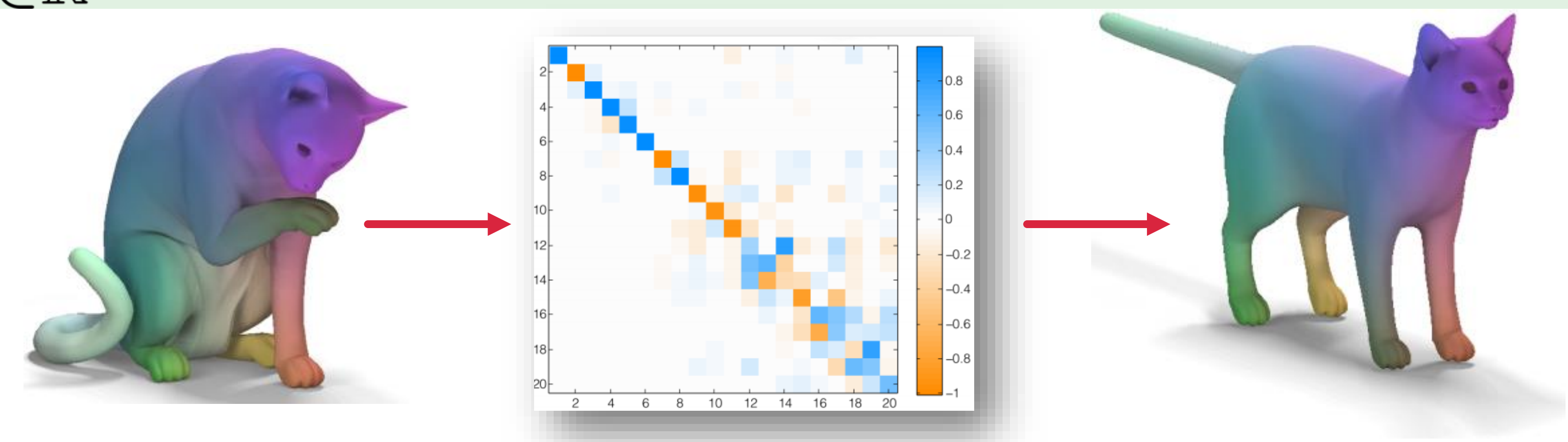
Roughly:

1. **Extract Laplace-Beltrami eigenfunctions:**

$$L\phi_i = \lambda_i A \phi_i$$

2. **Find mapping matrix (linear solve!):**

$$\min_{A \in \mathbb{R}^{n \times n}} \|AF_0 - F\|_{\text{Fro}}^2 + \alpha \|A\Delta_0 - \Delta A\|_{\text{Fro}}^2$$



Ovsjanikov et al. "Functional Maps." SIGGRAPH 2012.

Rough Plan

Part I (Justin)

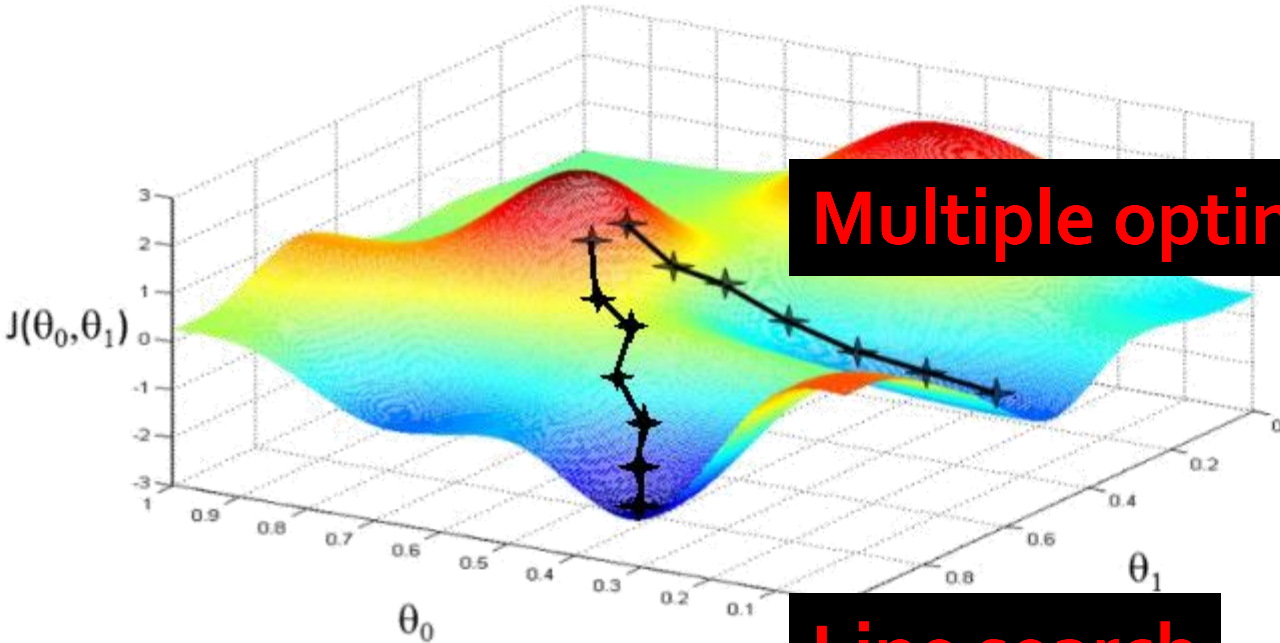
- Vocabulary
- Simple examples
- **Unconstrained optimization**
- Equality-constrained optimization

Unconstrained Optimization

$$\min_{x} f(x)$$

Unstructured.

Basic Algorithms



Multiple optima!

Line search

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k)$$

Gradient descent

Basic Algorithms

$$\lambda_0 = 0, \lambda_s = \frac{1}{2}(1 + \sqrt{1 + 4\lambda_{s-1}^2}), \gamma_s = \frac{1 - \lambda_2}{\lambda_{s+1}}$$

$$y_{s+1} = x_s - \frac{1}{\beta}\nabla f(x_s)$$

$$x_{s+1} = (1 - \gamma_s)y_{s+1} + \gamma_s y_s$$

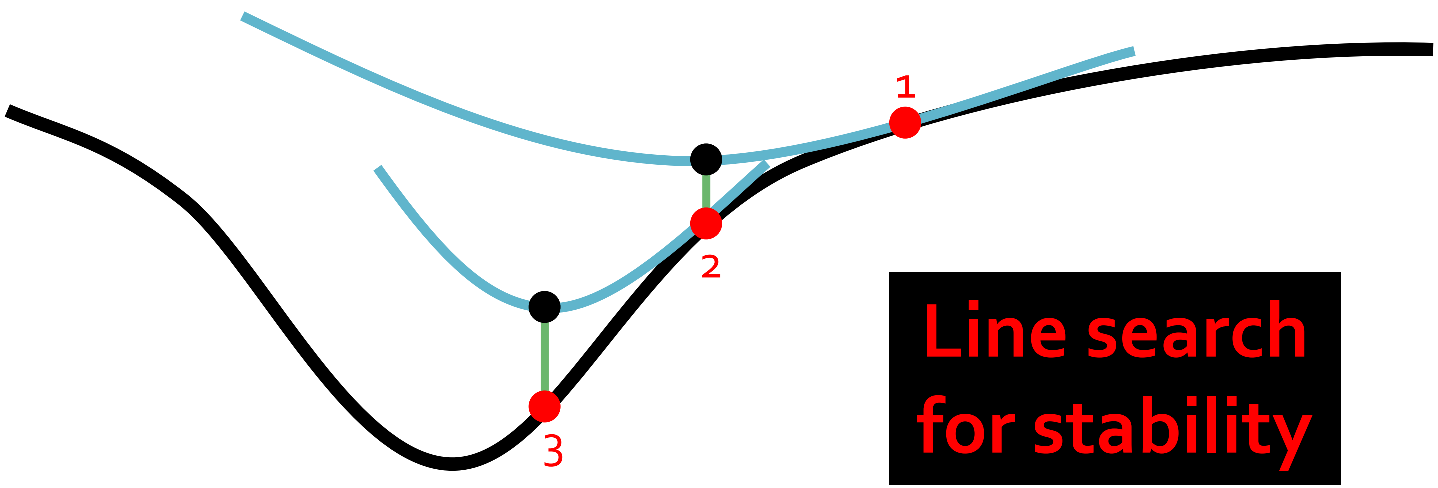
Quadratic convergence on convex problems!

(Nesterov 1983)

Accelerated gradient descent

Basic Algorithms

$$x_{k+1} = x_k - \boxed{[Hf(x_k)]^{-1}} \nabla f(x_k)$$



Line search for stability

Newton's Method

Basic Algorithms

$$x_{k+1} = x_k - \boxed{M_k^{-1}} \nabla f(x_k)$$

Hessian approximation

- (Often sparse) approximation from previous samples and gradients
- Inverse in closed form!

Quasi-Newton: BFGS and friends

Example: Shape Interpolation

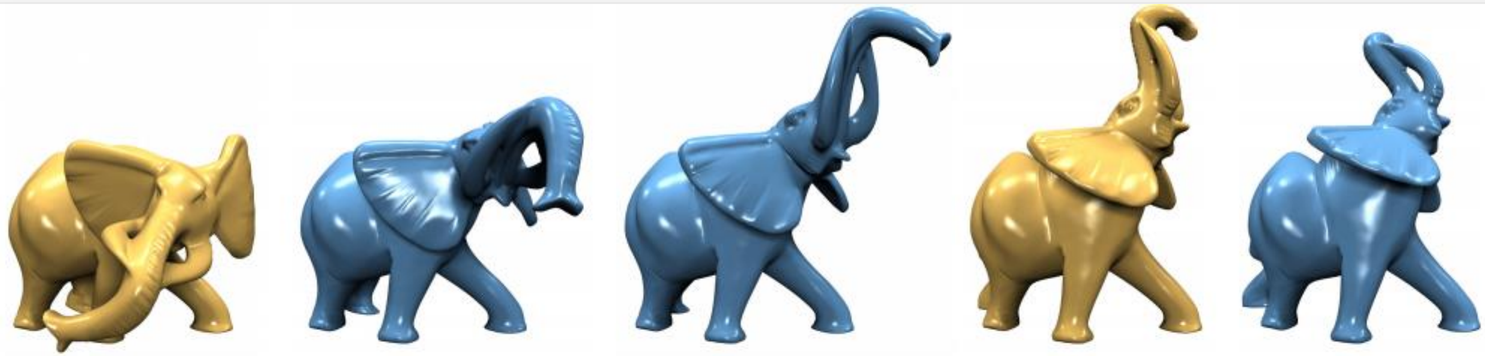


Figure 5: *Interpolation and extrapolation of the yellow example poses. The blending weights are* 0, 0.35, 0.65, 1.0, *and* 1.25.

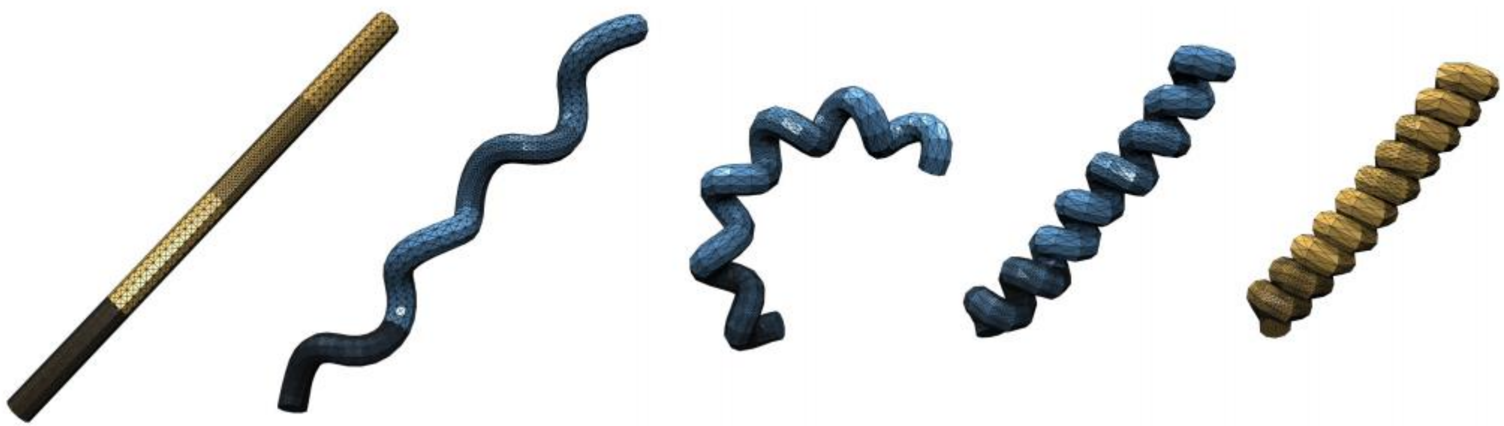


Figure 6: *Interpolation of an adaptively meshed and strongly twisted helix with blending weights* 0, 0.25, 0.5, 0.75, 1.0.

Fröhlich and Botsch. "Example-Driven Deformations Based on Discrete Shells." CGF 2011.

Interpolation Pipeline

Roughly:

1. **Linearly interpolate edge lengths and dihedral angles.**

$$\ell_e^* = (1-t)\ell_e^0 + t\ell_e^1$$

$$\theta_e^* = (1-t)\theta_e^0 + t\theta_e^1$$

2. **Nonlinear optimization for vertex positions.**

$$\min_{x_1,\ldots,x_m} \lambda \sum_e w_e(\ell_e(x) - \ell_e^*)^2$$

$$+ \mu \sum_e w_b(\theta_e(x) - \theta_e^*)^2$$

Sum of squares: Gauss-Newton

Software

- Matlab: `fminunc` or `minfunc`
- C++: `libLBFGS`, `dlib`, others

Typically provide functions for function and gradient (and optionally, Hessian).

Try several!

Some Tricks

Lots of small elements: $\|x\|_2^2 = \sum_i x_i^2$

Lots of zeros: $\|x\|_1 = \sum_i |x_i|$

Uniform norm: $\|x\|_\infty = \max_i |x_i|$

Low rank: $\|X\|_* = \sum_i \sigma_i$

Mostly zero columns: $\|X\|_{2,1} = \sum_j \sqrt{\sum_i x_{ij}^2}$

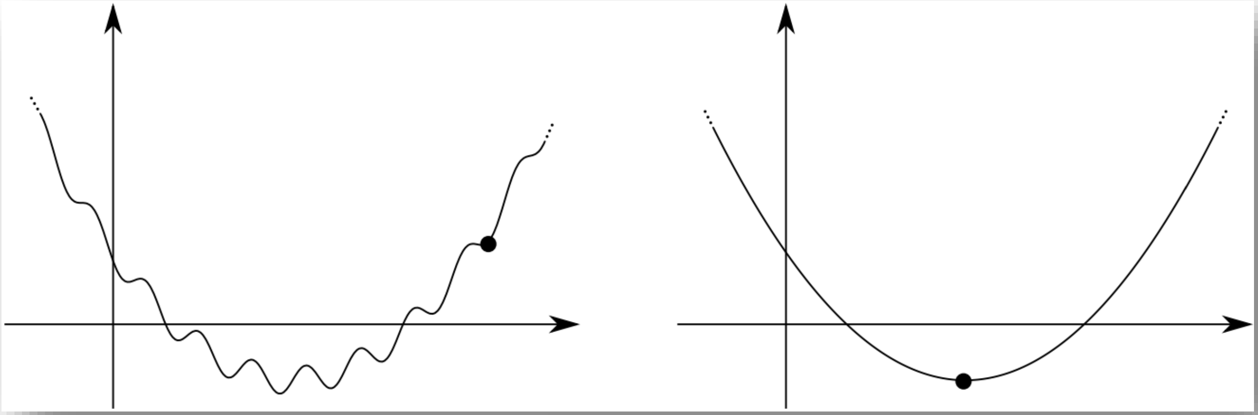
Smooth: $\int \|\nabla f\|_2^2$

Piecewise constant: $\int \|\nabla f\|_2$

???: Early stopping

Regularization

Some Tricks



Original Blurred

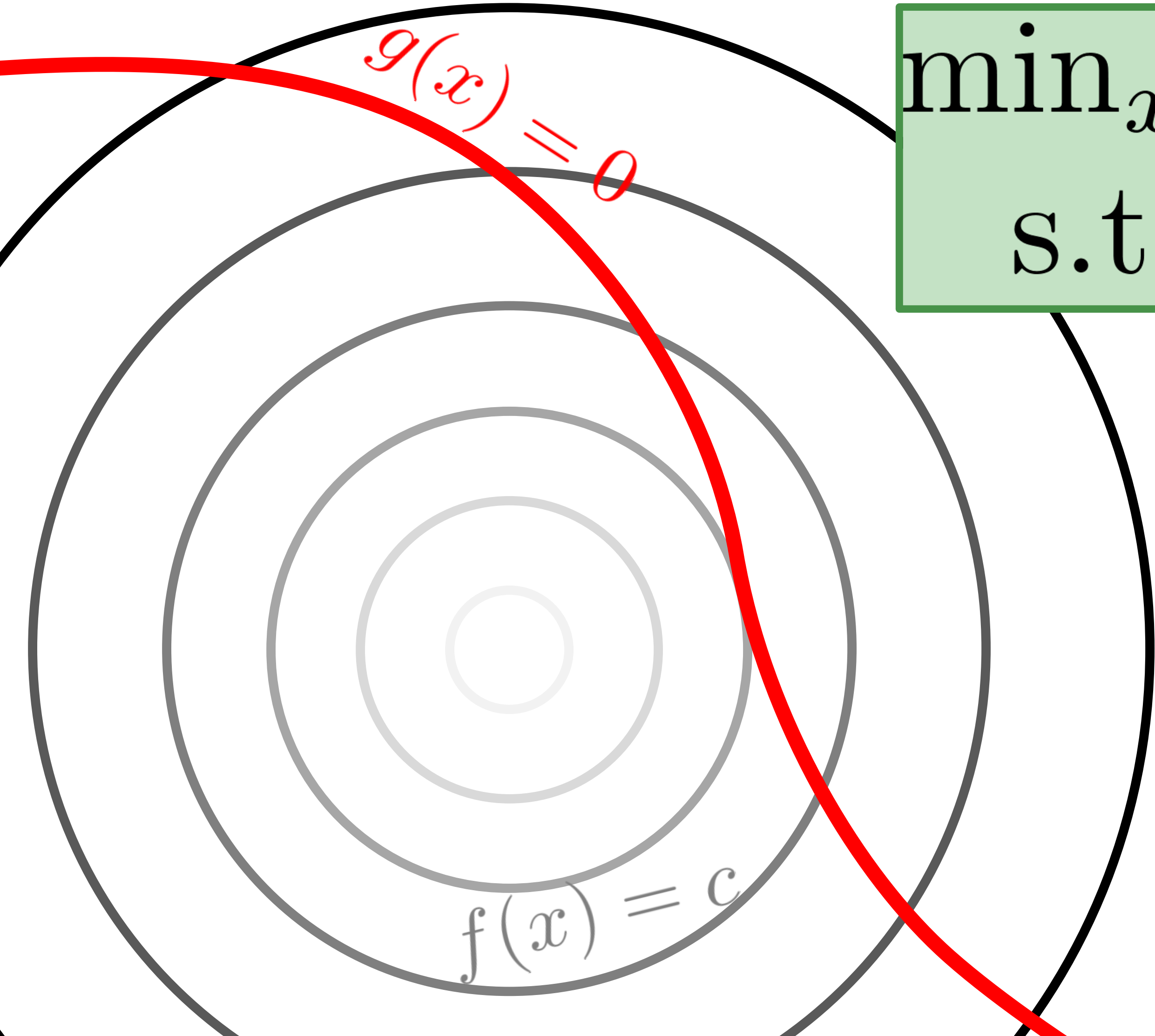
Multiscale/graduated optimization

Rough Plan

Part I (Justin)

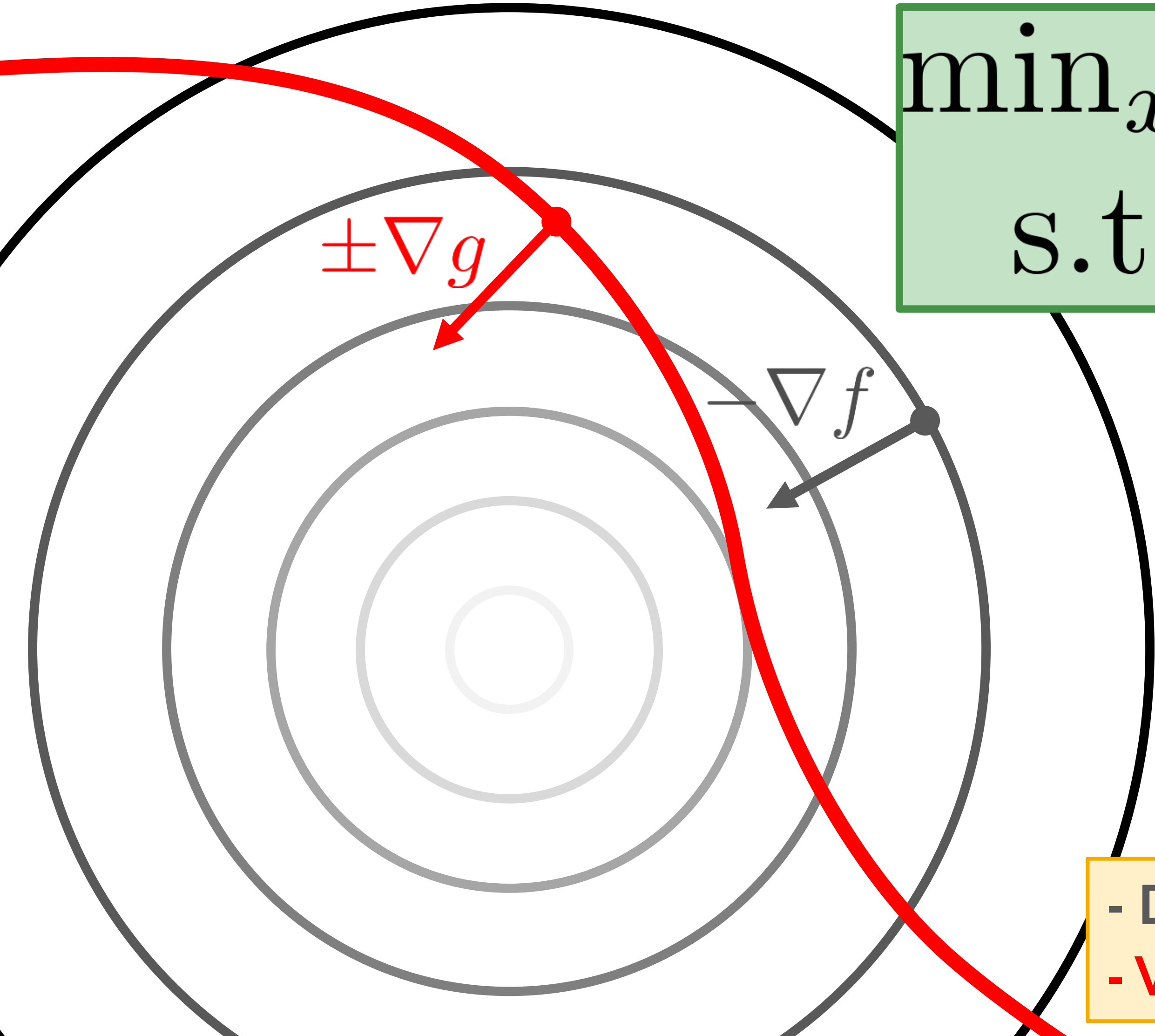
- Vocabulary
- Simple examples
- Unconstrained optimization
- **Equality-constrained optimization**

Lagrange Multipliers: Idea



$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

Lagrange Multipliers: Idea

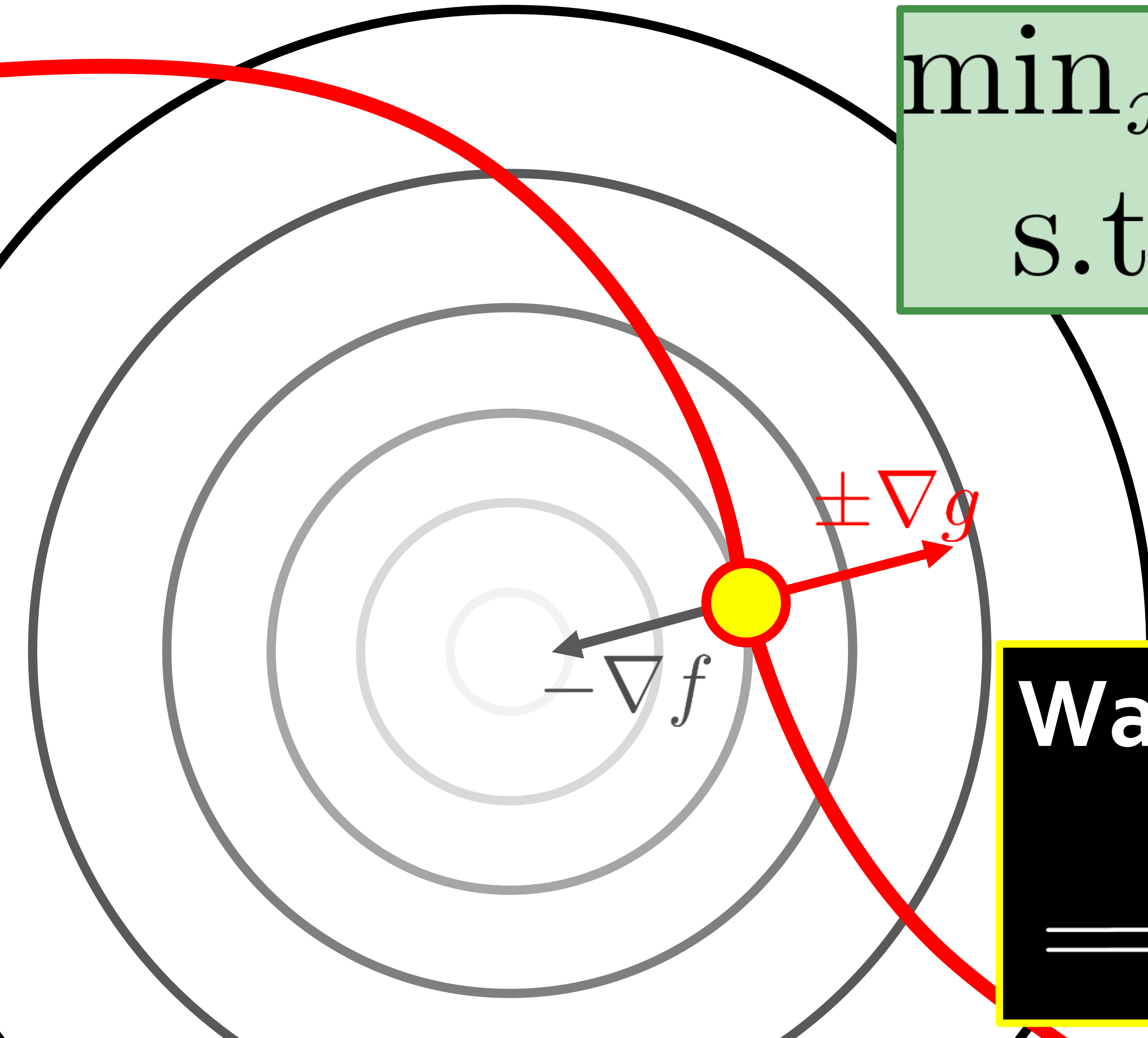


$$\min_x \quad f(x)$$
$$\text{s.t.} \quad g(x) = 0$$

- Decrease f: $-\nabla f$
- **Violate constraint: $\pm\nabla g$**

Lagrange Multipliers: Idea

$$\min_x \quad f(x)$$
$$\text{s.t.} \quad g(x) = 0$$



Want:

$$\nabla f \| \nabla g$$

$$\Longrightarrow \quad \nabla f = \lambda \nabla g$$

Example: Symmetric Eigenvectors

$$f(x) = x^\top Ax \implies \nabla f(x) = 2Ax$$

$$g(x) = \|x\|_2^2 \implies \nabla g(x) = 2x$$

$$\implies Ax = \lambda x$$

Use of Lagrange Multipliers

Turns constrained optimization into

unconstrained root-finding.

$$\nabla f(x) = \lambda \nabla g(x)$$

$$g(x) = 0$$

Many Options

- **Reparameterization**

  Eliminate constraints to reduce to unconstrained case

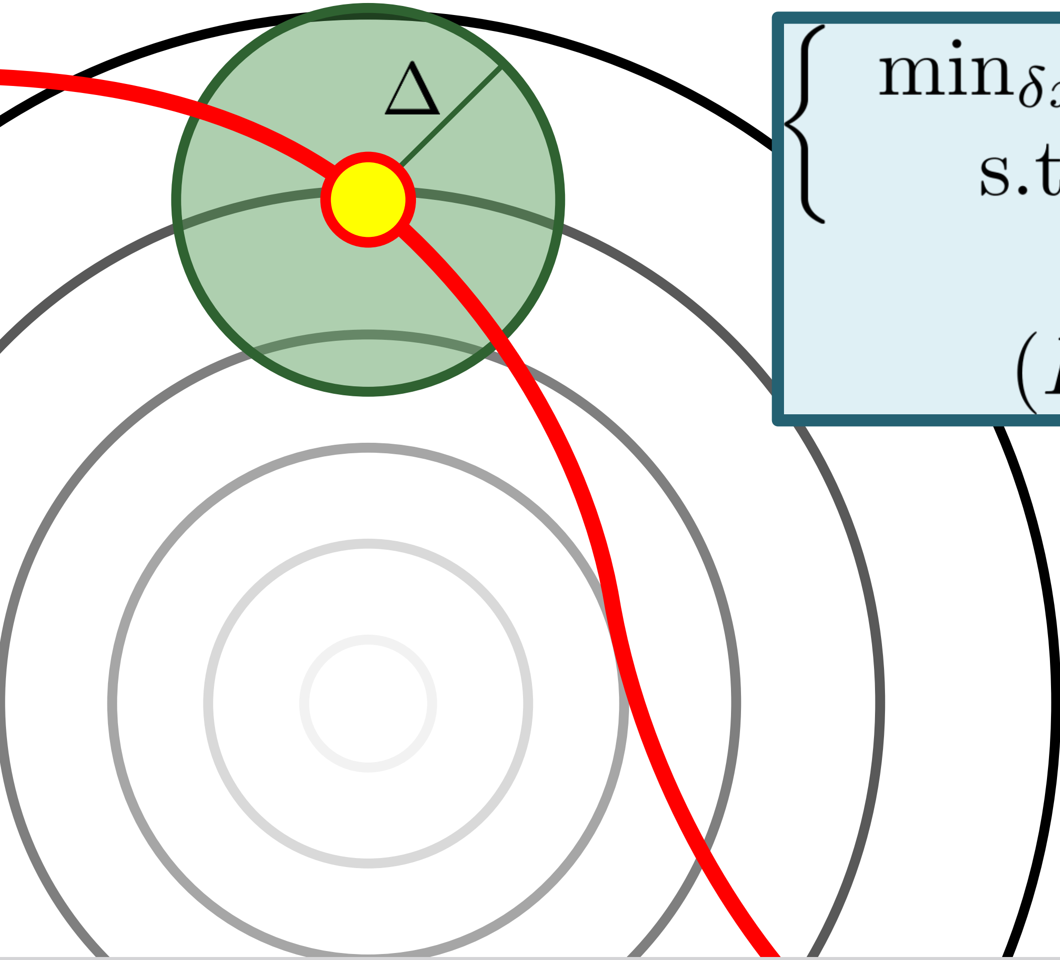
- **Newton's method**

  Approximation: quadratic function with linear constraint

- **Penalty method**

  Augment objective with barrier term, e.g. $f(x) + \rho|g(x)|$

Trust Region Methods



$$\left\{\begin{array}{ll} \min_{\delta x} & \frac{1}{2}\delta x^\top H \delta x + w^\top x \\ \text{s.t.} & \|\delta x\|_2^2 \leq \Delta \end{array}\right\}$$

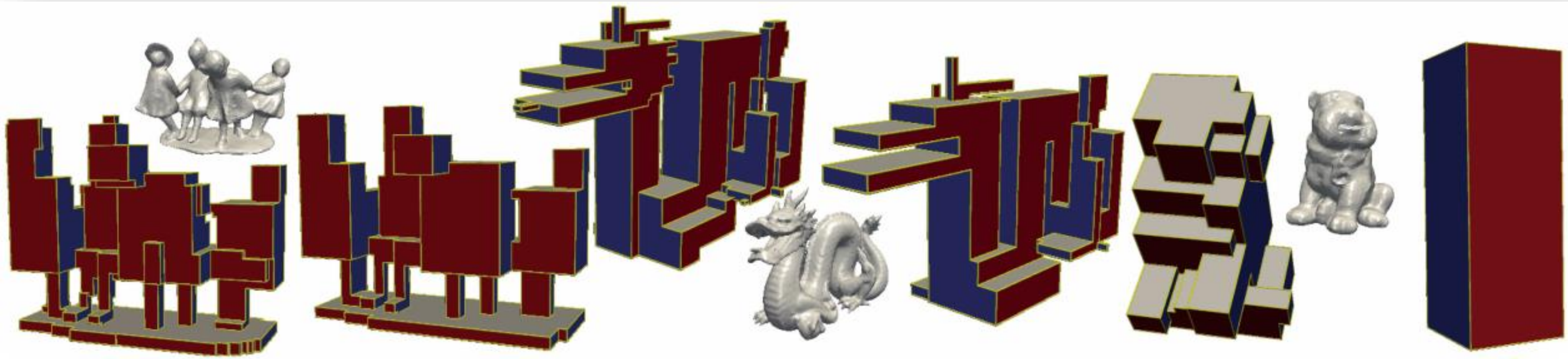
$$\downarrow$$

$$(H + \lambda I)\delta x = -w$$

Fix (or adjust) *damping parameter* $\lambda > 0$.

Example: Levenberg-Marquardt

Example: Polycube Maps



Huang et al. "L1-Based Construction of Polycube Maps from Complex Shapes." TOG 2014.

Align with coordinate axes

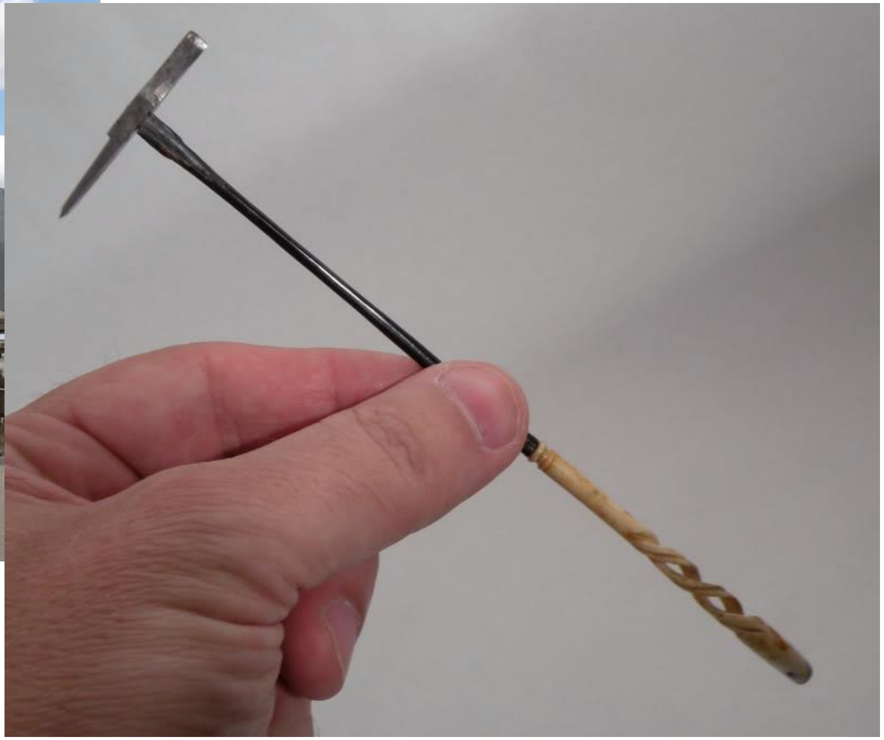
$$\begin{aligned} \min_X \textstyle\sum_{b_i} \quad & A(b_i;X)\|n(b_i;X)\|_1 \\ \text{s.t.} \quad & \textstyle\sum_{b_i} A(b_i;X) = \sum_{b_i} A(b_i;X_0) \end{aligned}$$

Preserve area

Note: Final method includes more terms!

Convex Optimization Tools

versus

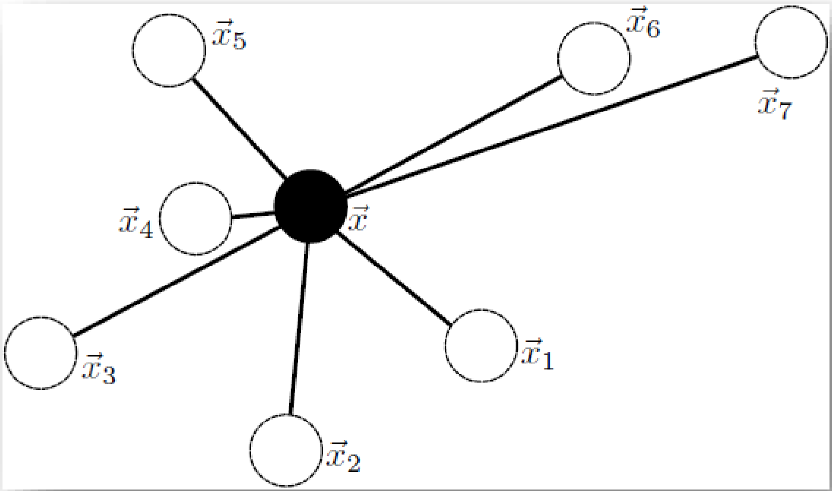


Sometimes work for non-convex problems...

Try lightweight options

Iteratively Reweighted Least Squares

$$\min_x \sum_i \phi(x \top a_i + b_i) \leftrightarrow \begin{Bmatrix} \min_{x,y_i} & \sum_i y_i (x^\top a_i + b_i)^2 \\ \text{s.t.} & y_i = \phi(x^\top a_i + b_i)(x^\top a_i + b_i)^{-2} \end{Bmatrix}$$



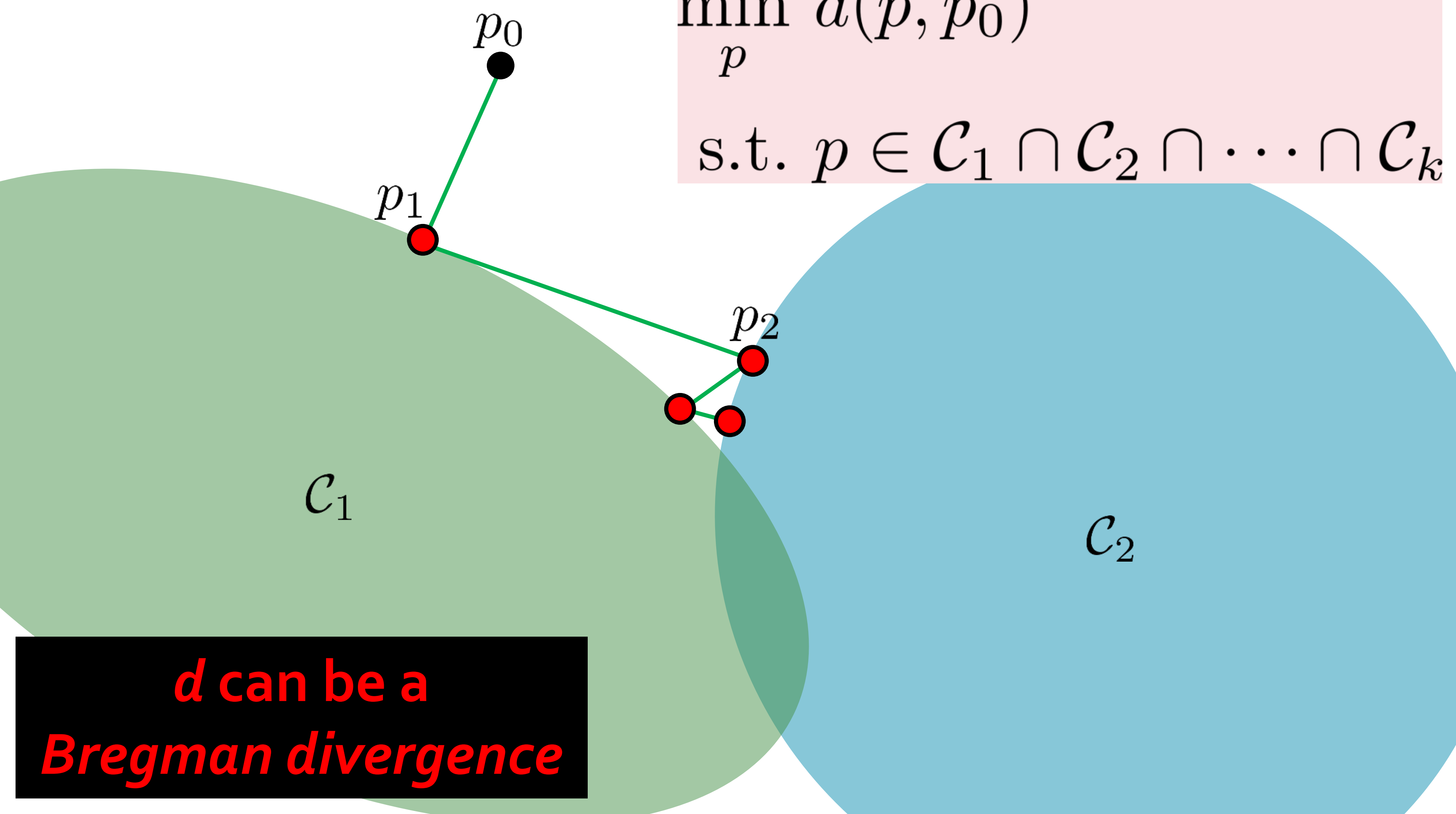
"Geometric median"

$$\min_x \sum_i \|x - p_i\|_2 \implies \begin{cases} x & \leftarrow \min_x \sum_i y_i \|x - p_i\|_2^2 \\ y_i & \leftarrow \|x - p_i\|_2^{-1} \end{cases}$$

Repeatedly solve linear systems

Alternating Projection

$$\min_p \; d(p, p_0)$$
$$\text{s.t. } p \in \mathcal{C}_1 \cap \mathcal{C}_2 \cap \cdots \cap \mathcal{C}_k$$



d* can be a *Bregman divergence

Iterative Shrinkage-Thresholding

$$x_{t+1} = x_t - \eta \nabla f(x_t)$$

$$\iff x_{t+1} = \arg\min_x \left[f(x_t) + \nabla f(x_t)^\top (x - x_t) + \frac{1}{2\eta} \|x - x_t\|_2^2 \right]$$

$$\iff x_{t+1} = \arg\min_x \frac{1}{2\eta} \|x - (x_t - \eta \nabla f(x_t))\|_2^2$$

Decompose as sum of hard part *f* and easy part *g*.

To minimize $f(x) + g(x)$:

$$x_{t+1} = \arg\min_x \left[g(x) + \tfrac{1}{2\eta} \|x - (x_t - \eta \nabla f(x_t))\|_2^2 \right]$$

FISTA combines with Nesterov descent!

https://blogs.princeton.edu/imabandit/2013/04/11/orf523-ista-and-fista/

Augmented Lagrangians

$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

$$\downarrow$$

$$\begin{aligned} \min_x \quad & f(x) + \frac{\rho}{2}\|g(x)\|_2^2 \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

Does nothing when constraint is satisfied

Add constraint to objective

Alternating Direction Method of Multipliers (ADMM)

$$\begin{aligned} \min_{x,z} \quad & f(x) + g(z) \\ \text{s.t.} \quad & Ax + Bz = c \end{aligned}$$

$$\Lambda_\rho(x, z; \lambda) = f(x) + g(z) + \lambda^\top (Ax + Bz - c) + \frac{\rho}{2}\|Ax + Bz - c\|_2^2$$

$$x \leftarrow \arg\min_x \Lambda_\rho(x, z, \lambda)$$

$$z \leftarrow \arg\min_z \Lambda_\rho(x, z, \lambda)$$

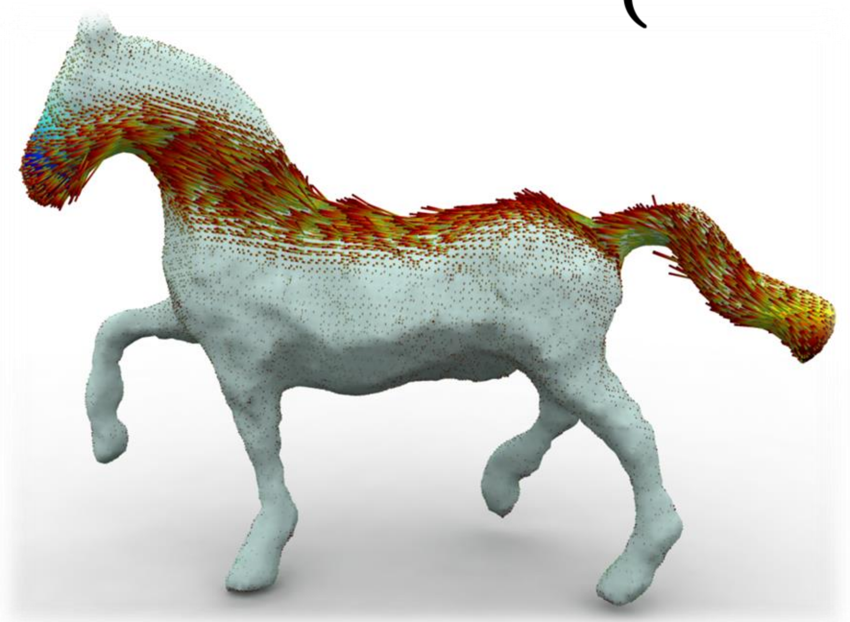
$$\lambda \leftarrow \lambda + \rho(Ax + Bz - c)$$

https://web.stanford.edu/~boyd/papers/pdf/admm_slides.pdf

The Art of ADMM "Splitting"

$$\left\{\begin{array}{rl}\min_J & \sum_i \|J_i\|_2\\ \text{s.t.} & MJ=b\end{array}\right\} \longrightarrow \left\{\begin{array}{rl}\min_{J,\bar J} & \sum_i \left(\|J_i\|_2 + \frac{\rho}{2}\|J_i-\bar J_i\|_2^2\right)\\ \text{s.t.} & M\bar J = b\\ & J=\bar J\end{array}\right\}$$

Augmented part



Takes some practice!
Example of "proximal" algorithm.

Solomon et al. "Earth Mover's Distances on Discrete Surfaces." SIGGRAPH 2014.

Want two *easy* subproblems

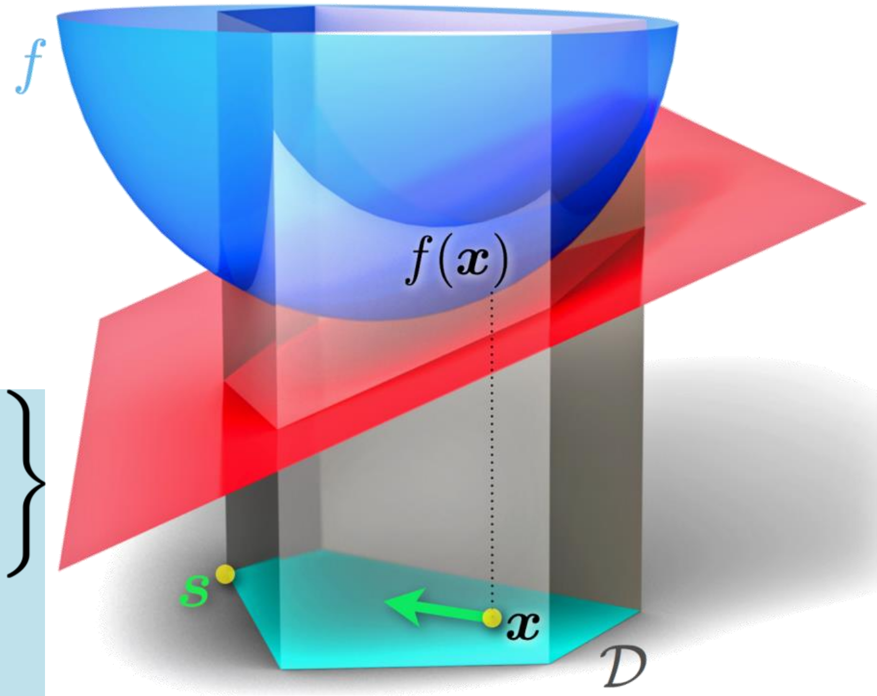
Frank-Wolfe

To minimize $f(x)$ s.t. $x \in \mathcal{D}$:

$$s_k \leftarrow \left\{ \begin{array}{c} \arg\min_s \quad s^\top \nabla f(x_k) \\ \text{s.t.} \quad s \in \mathcal{D} \end{array} \right\}$$

$$\gamma \leftarrow \frac{2}{k+2}$$

$$x_{k+1} \leftarrow x_k + \gamma(s_k - x_k)$$



https://en.wikipedia.org/wiki/Frank%E2%80%93Wolfe_algorithm

Linearize objective, preserve constraints