IFT 6113 BACKGROUND: LINEAR ALGEBRA AND OPTIMIZATION

http://tiny.cc/ift6113



Mikhail Bessmeltsev

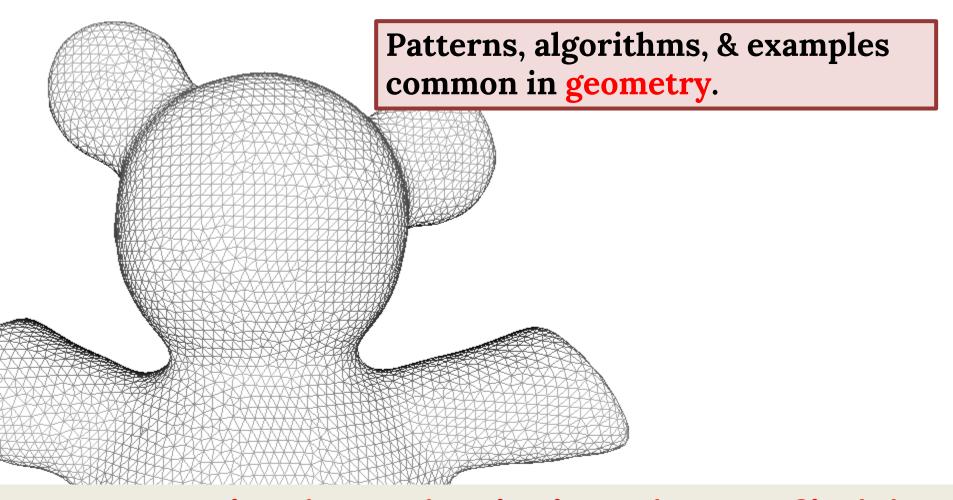
MOTIVATION

Numerical problems are everywhere in geometric modeling!

Quick summary!

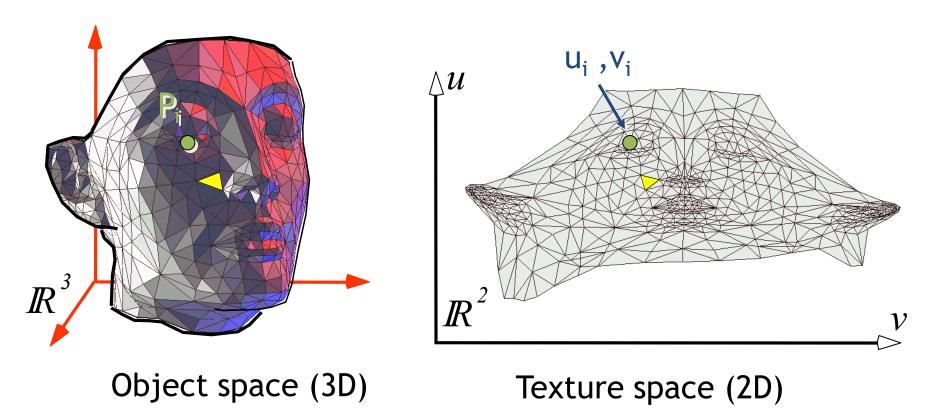
Mostly for common ground: You may already know this material. First half is important; remainder summarizes interesting recent tools.

OUR BIAS



Numerical analysis is a <u>huge</u> field.

How to flatten a mesh?





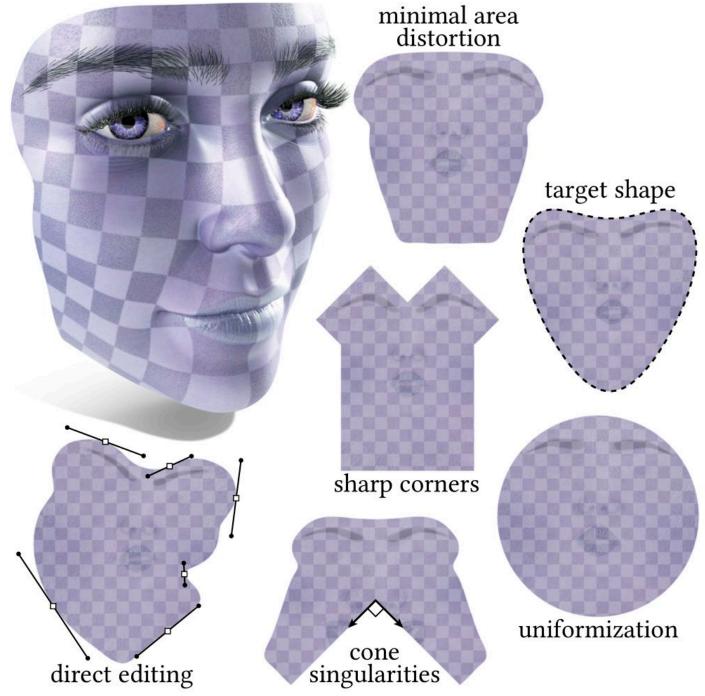
How to flatten a mesh?

$$\min_{u_i,v_i\in\mathbb{R}^2} f(u_1,v_1,\ldots,u_n,v_n)$$

Fit a target 2D shape?

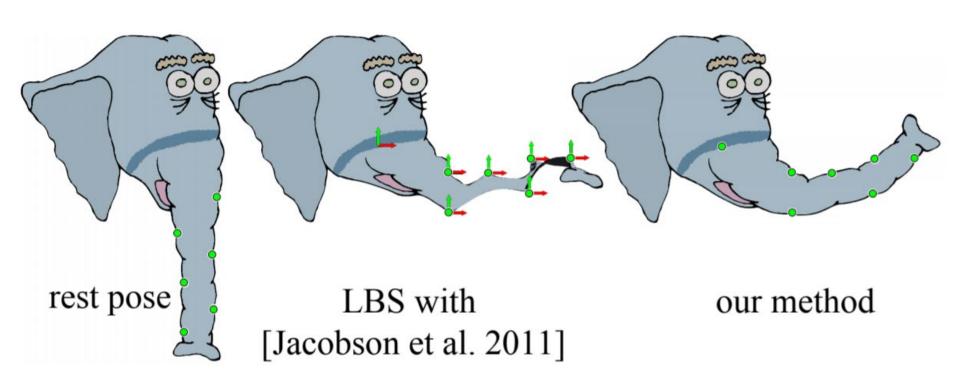
Triangle distortion?

More sharp corners?



"Boundary First Flattening" by Rohan Sawhney and Keenan Crane

How to animate a character?



How to animate a character?

$$\min_{\substack{x_i, y_i \in \mathbb{R}^2}} f(x_1, y_1, \dots, x_n, y_n)$$
s.t. $x_j - x_j' = 0$

$$y_j - y_j' = 0$$
Known positions

Triangle distortion?

Some smoothness?

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

$$h(x) \ge 0$$

Optimized function (Energy)

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

$$h(x) \ge 0$$

$$\min_{x \in \mathbb{R}^n} f(x)$$

Equality constraints

s.t.
$$g(x) = 0$$

 $h(x) \ge 0$

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

$$h(x) \ge 0$$

Inequality constraints

$$Ax = b \qquad \Leftrightarrow \quad \min_{x \in \mathbb{R}^n} ||Ax - b||_2^2$$

$$Ax = \lambda x \quad \leftrightarrow \quad \frac{\min_{x \in \mathbb{R}^n} ||Ax||_2^2}{\text{s.t. } ||x|| - 1 = 0}$$

ROUGH PLAN

- (intro) Matrices and Eigenvalues
- Linear problems
- Unconstrained optimization
- Equality-constrained optimization
- Variational problems

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How are those matrices special?

$$\begin{pmatrix} 1 & & & \\ & -2 & & \\ & & 5 \end{pmatrix} \qquad \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 5 \end{pmatrix} \qquad \begin{pmatrix} 0 & -1 & -2 \\ 1 & 0 & 4 \\ 2 & -4 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$

$$\begin{pmatrix} 0 & -1 & -2 \\ 1 & 0 & 4 \\ 2 & -4 & 0 \end{pmatrix}$$

$$\begin{pmatrix}
\cos(0.4) & -\sin(0.4) & 0 \\
\sin(0.4) & \cos(0.4) & 0 \\
0 & 0 & 1
\end{pmatrix} \qquad \begin{pmatrix}
1 & 0 & 3 \\
0 & 1 & 4 \\
& & 1
\end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 3 \\ 0 & 1 & 4 \\ & & 1 \end{pmatrix}$$

How are those matrices special?

$$\begin{pmatrix} 1 & & \\ & -2 & \\ & & 5 \end{pmatrix}$$

Diagonal

$$\begin{pmatrix} 1 & & & \\ & -2 & & \\ & & 5 \end{pmatrix} \qquad \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 5 \end{pmatrix} \qquad \begin{pmatrix} 0 & -1 & -2 \\ 1 & 0 & 4 \\ 2 & -4 & 0 \end{pmatrix}$$

Symmetric $A = A^T$

$$\begin{pmatrix} 0 & -1 & -2 \\ 1 & 0 & 4 \\ 2 & -4 & 0 \end{pmatrix}$$

Skew-symmetric $A^T = -A$

$$\begin{pmatrix}
\cos(0.4) & -\sin(0.4) & 0 \\
\sin(0.4) & \cos(0.4) & 0 \\
0 & 0 & 1
\end{pmatrix}$$

Orthogonal $A^{-1} = A^T$

$$\begin{pmatrix} 1 & 0 & 3 \\ 0 & 1 & 4 \\ & & 1 \end{pmatrix}$$

Um something?

What is the geometric meaning of those?

$$\begin{pmatrix} 1 & & \\ & -2 & \\ & & 5 \end{pmatrix}$$

Diagonal

$$\begin{pmatrix}
\cos(0.4) & -\sin(0.4) & 0 \\
\sin(0.4) & \cos(0.4) & 0 \\
0 & 0 & 1
\end{pmatrix}$$

Orthogonal
$$A^{-1} = A^T$$

$$\begin{pmatrix} 1 & 0 & 3 \\ 0 & 1 & 4 \\ & & 1 \end{pmatrix}$$

Um something?

INTRO TO INTRO

What is the geometric meaning of those?

$$\begin{pmatrix} 1 & & \\ & -2 & \\ & & 5 \end{pmatrix}$$

Non-uniform scaling

$$\begin{pmatrix}
\cos(0.4) & -\sin(0.4) & 0 \\
\sin(0.4) & \cos(0.4) & 0 \\
0 & 0 & 1
\end{pmatrix}$$

Rotation

$$\begin{pmatrix} 1 & 0 & 3 \\ 0 & 1 & 4 \\ & & 1 \end{pmatrix}$$

Translation in 2D*

DIAGONAL MATRICES

- Those are the eigenvalues!
- Scaling along coordinate axes
- $\Theta(n)$ space to store (just *n* of course)
- O(n) time to invert

$$\begin{pmatrix} 1 & & \\ & -2 & \\ & & 5 \end{pmatrix}$$
 Diagonal

SYMMETRIC MATRICES

- All eigenvalues are real
- All eigenvectors are orthogonal

Can be diagonalized by an orthogonal matrix: $D = Q^{T} A Q$

$$\begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$
Symmetric
$$A = A^{T}$$

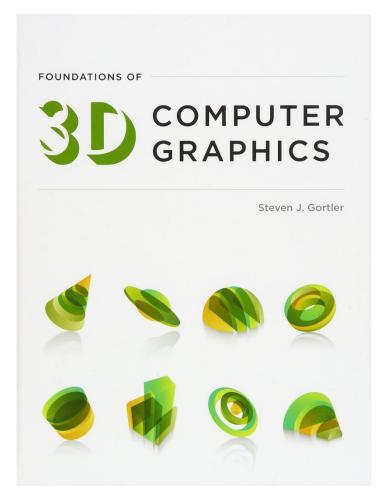
ORTHOGONAL MATRICES

- $AA^T = I$
- Columns have zero dot product
- Doesn't change length of vectors or angles between them (isometry)
- Determinant is ±1

$$\begin{pmatrix}
\cos(0.4) & -\sin(0.4) & 0 \\
\sin(0.4) & \cos(0.4) & 0 \\
0 & 0 & 1
\end{pmatrix}$$
Orthogonal

$$A^{-1} = A^T$$

NO IDEA WHAT THOSE ARE?



https://umontreal.on.worldcat.org/oclc/829434522
Free online at UdeM library
Chapters I.3, I.4

Eigenvalues and eigenvectors

$$Ax = \lambda x$$

discrete

or

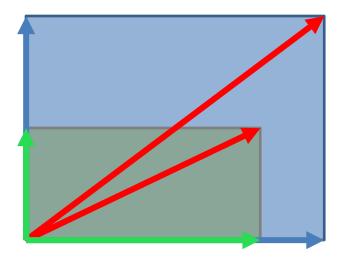
$$\mathcal{L}[f(x)] = \lambda f(x)$$
 continuous

- Geometric transformations
- Linear operators on (discrete) functions

EIGENVECTORS/VALUES

Geometric meaning?

Vectors which **only** scale



MATRIX IS POSITIVE DEFINITE

$$A \geqslant 0$$



All eigenvalues are nonnegative

Geometric meaning?

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

$$h(x) \ge 0$$

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VECTOR SPACES AND LINEAR OPERATORS

$$\mathcal{L}[\vec{x} + \vec{y}] = \mathcal{L}[\vec{x}] + \mathcal{L}[\vec{y}]$$

$$\mathcal{L}[c\vec{x}] = c\mathcal{L}[\vec{x}]$$

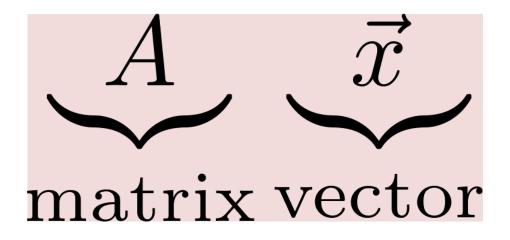
ABSTRACT EXAMPLE

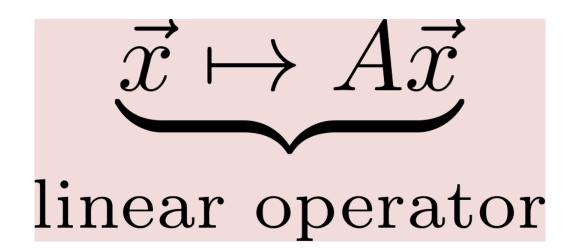
$$C^{\infty}(\mathbb{R})$$

$$\mathcal{L}[f] := df/dx$$

Eigenvectors?

IN FINITE DIMENSIONS





LINEAR SYSTEM OF EQUATIONS

$$\left(\begin{array}{c}A\end{array}\right)\left(\vec{x}\right)=\left(\vec{b}\right)$$

Simple "inverse problem"

COMMON STRATEGIES

- Gaussian elimination
 - $O(n^3)$ time to solve Ax=b or to invert
- **But:** Inversion is unstable and slower!

• Never ever compute A⁻¹ if you can avoid it.

SIMPLE EXAMPLE

$$\frac{d^2f}{dx^2} = g, f(0) = f(1) = 0$$

$$\begin{pmatrix} -2 & 1 & & & & & \\ 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & & & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{pmatrix}$$

STRUCTURE?

$$\begin{pmatrix}
-2 & 1 \\
1 & -2 & 1 \\
& 1 & -2 & 1
\end{pmatrix}$$

$$\vdots$$

$$1 & -2 & 1 \\
& 1 & -2$$

LINEAR SOLVER CONSIDERATIONS

- Never construct A^{-1} explicitly (if you can avoid it)
- Added structure helps
 Sparsity, symmetry, positive definiteness, bandedness

$$inv(A)*b \ll (A'*A) \setminus (A'*b) \ll A \setminus b$$

LINEAR SYSTEMS: SOLVERS

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

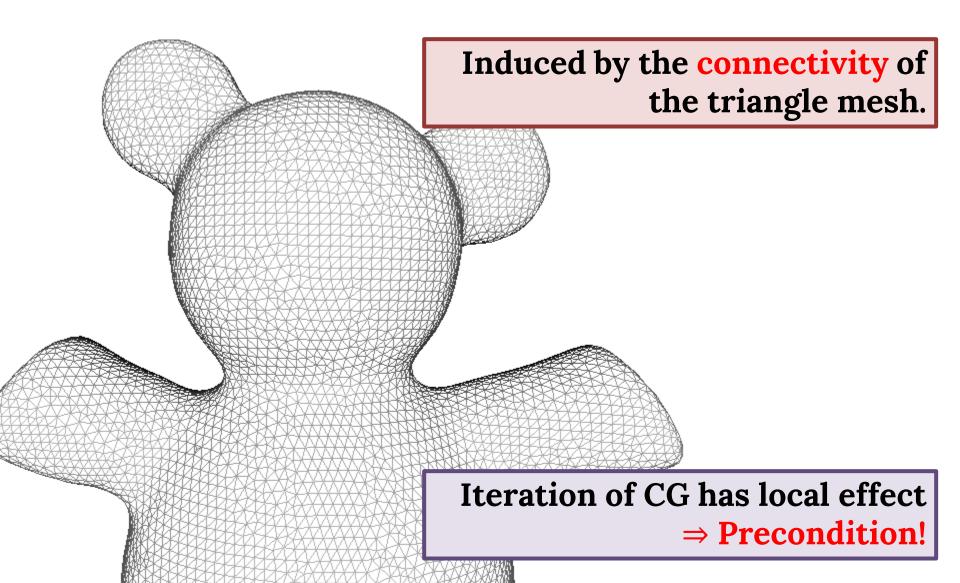
GENERIC ADVICE

Generic tools are often not too effective!

GENERIC ADVICE

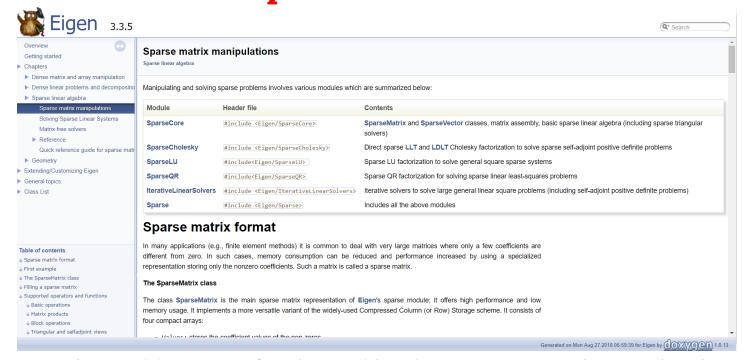
Try the simplest solver first.

VERY COMMON: SPARSITY



FOR IFT 6113

- No need to implement a linear solver
- If a matrix is sparse, your code should store it as a sparse matrix!



ROUGH PLAN

- (intro) Matrices and Eigenvalues
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- Variational problems

UNCONSTRAINED OPTIMIZATION

$$\min_{x \in \mathbb{R}^n} f(x)$$

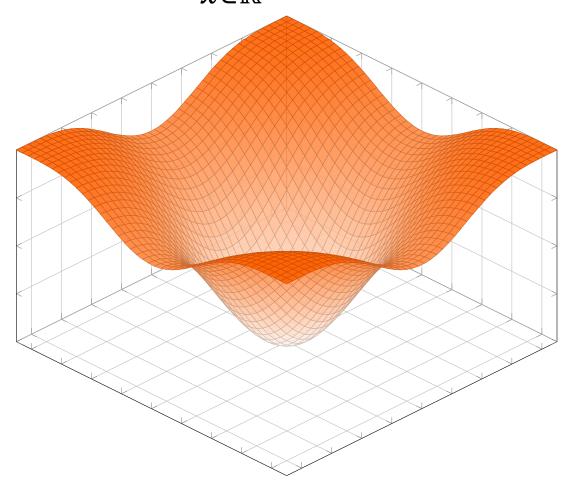
Trivial when f(x) is linear

Easy when f(x) is quadratic

Hard in case of generic non-linear.

UNCONSTRAINED OPTIMIZATION

 $\min_{x\in\mathbb{R}^n} f(x)$



$$f(x,y) = 3x^{2} - y$$

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (6x, -1)$$

Geometric meaning?

Gradient

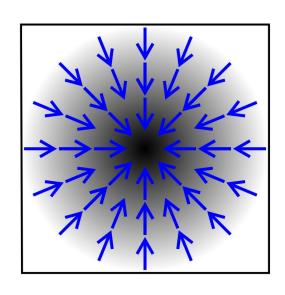
$$f: \mathbb{R}^n \to \mathbb{R}$$

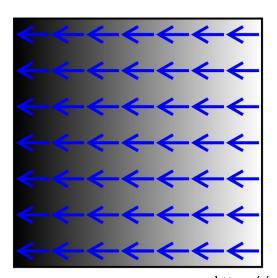
$$\rightarrow \nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n}\right)$$

Gradient

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

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





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

Gradient

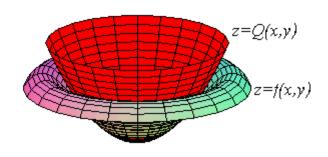
$$f: \mathbb{R}^n \to \mathbb{R}^m$$

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

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

Jacobian

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

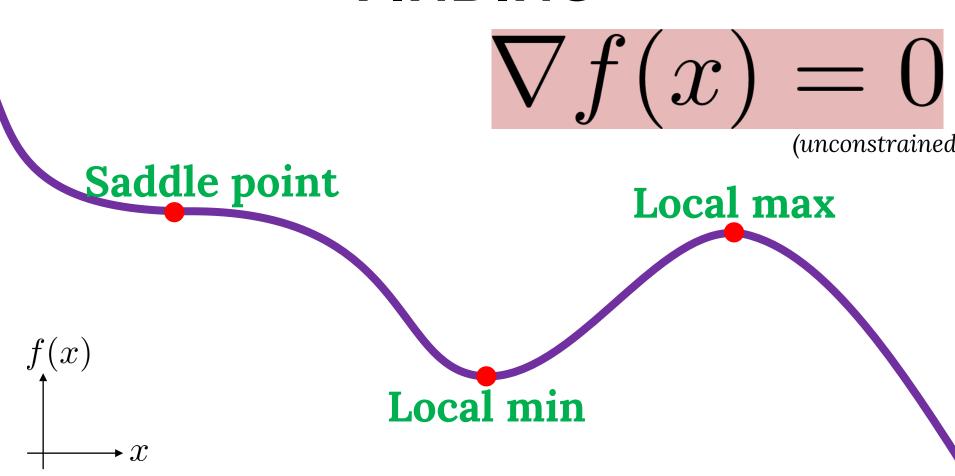


$$f(x) \approx f(x_0) + \nabla f(x_0)^{\top} (x - x_0) + (x - x_0)^{\top} H f(x_0) (x - x_0)$$

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

Hessian

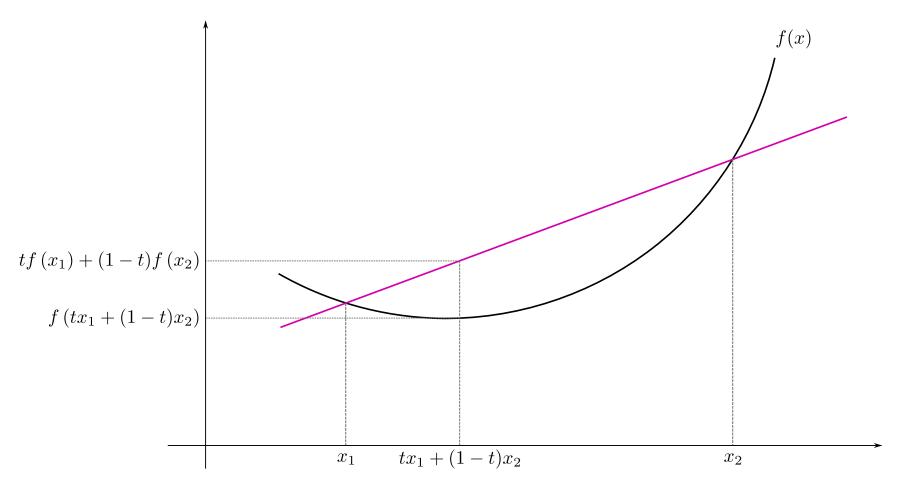
OPTIMIZATION TO ROOT-FINDING



Critical point

CONVEX FUNCTIONS

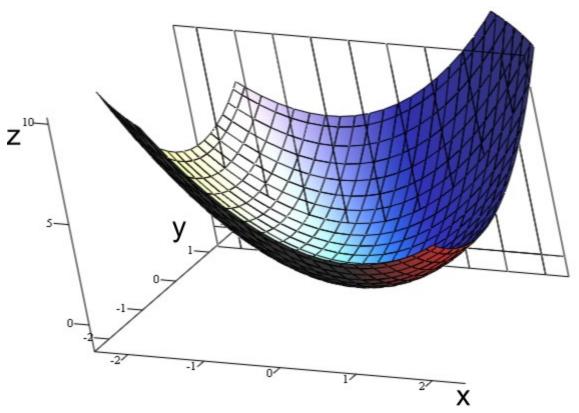
 $f^{\prime\prime}(x)>0$



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

CONVEX FUNCTIONS

$$H(x) \geqslant 0$$



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

SPECIAL CASE: LEAST-SQUARES

$$\min_{x} \frac{1}{2} ||Ax - b||_{2}^{2}$$

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

$$\implies A^{\top}Ax = A^{\top}b$$

Normal equations (better solvers for this case!)

USEFUL DOCUMENT

The Matrix Cookbook

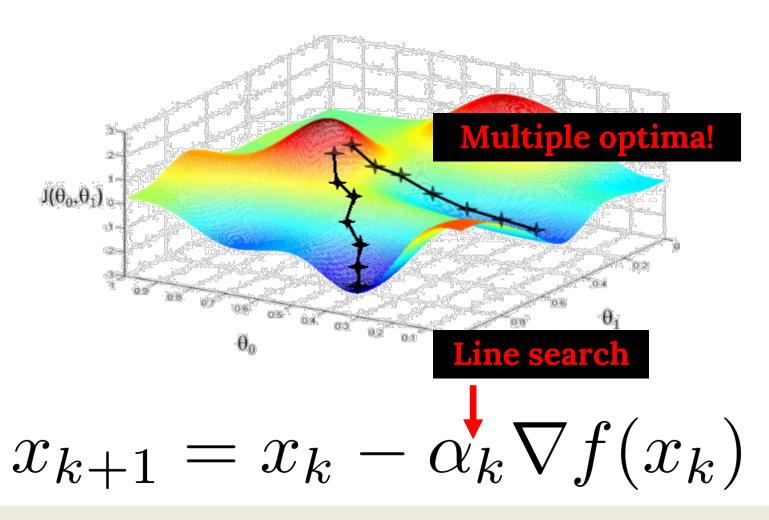
Petersen and Pedersen

http://www2.imm.dtu.dk/pubdb/views/edoc_download.php/3274/pdf/imm3274.pdf

UNCONSTRAINED OPTIMIZATION

$$\min f(x)$$

$$\mathcal{X}$$
Unstructured.



Gradient descent

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

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

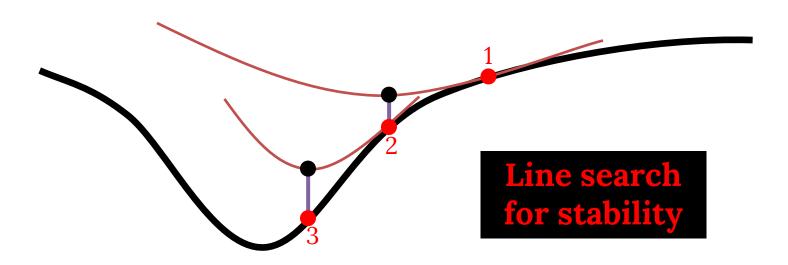
$$x_{s+1} = (1 - \gamma_s)y_{s+1} + \gamma_s y_s$$

Quadratic convergence on convex problems! (Nesterov 1983)

A very cool intro: https://distill.pub/2017/momentum/

Accelerated gradient descent

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



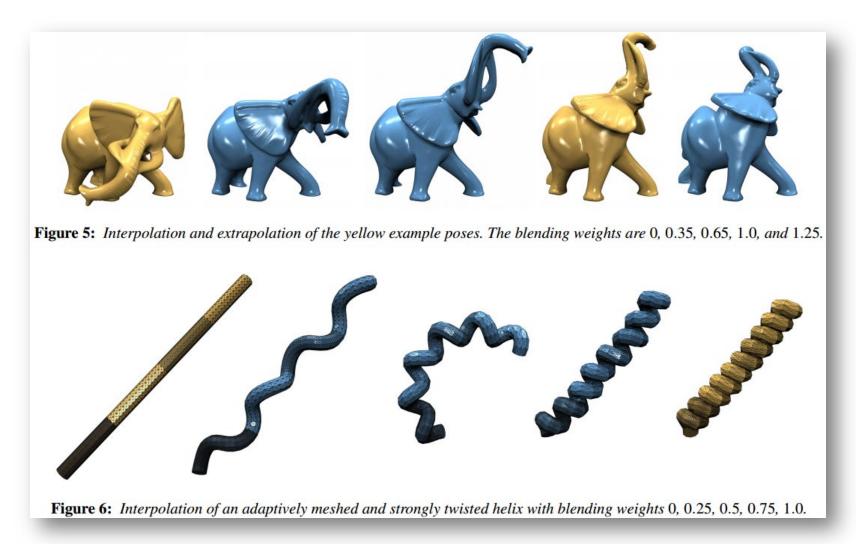
Newton's Method

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

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

Quasi-Newton: BFGS and friends

EXAMPLE: SHAPE INTERPOLATION



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

INTERPOLATION PIPELINE

Roughly:

1. Linearly interpolate edge lengths and dihedral angles.

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

2. Nonlinear optimization for vertex positions.

$$\min_{x_1, \dots, x_m} \lambda \sum_{e} w_e (\ell_e(x) - \ell_e^*)^2$$

Sum of squares: Gauss-Newton

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

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

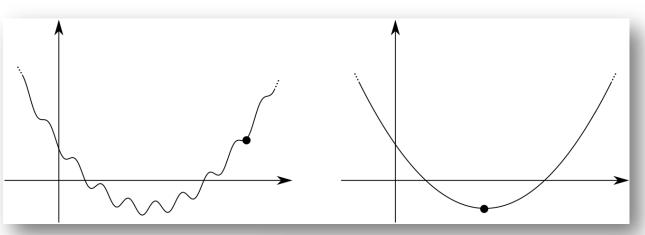
Mostly zero columns:
$$||X||_{2,1} = \sum_{j} \sqrt{\sum_{i} x_{ij}^2}$$

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

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

Regularization

SOME TRICKS





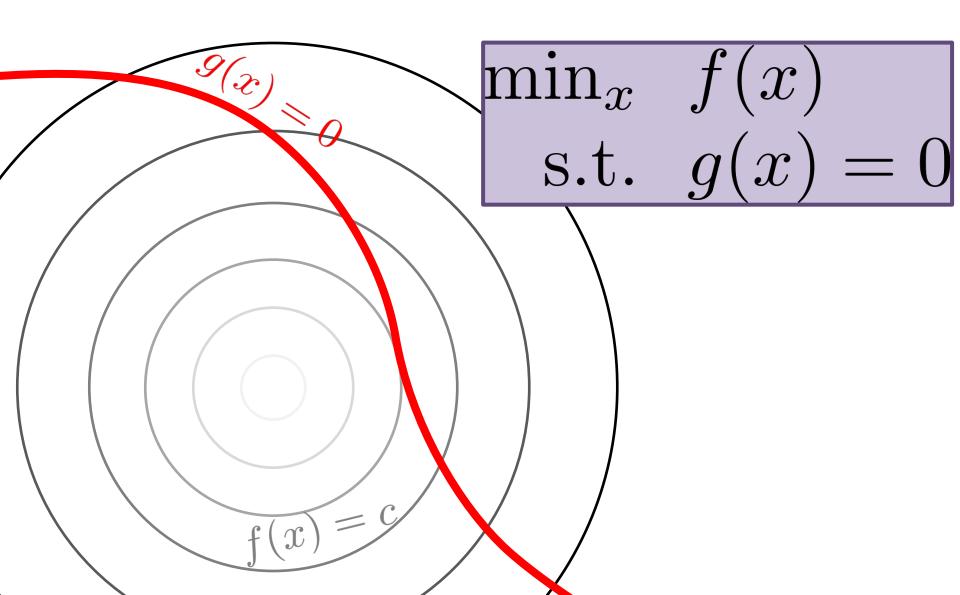


Multiscale/graduated optimization

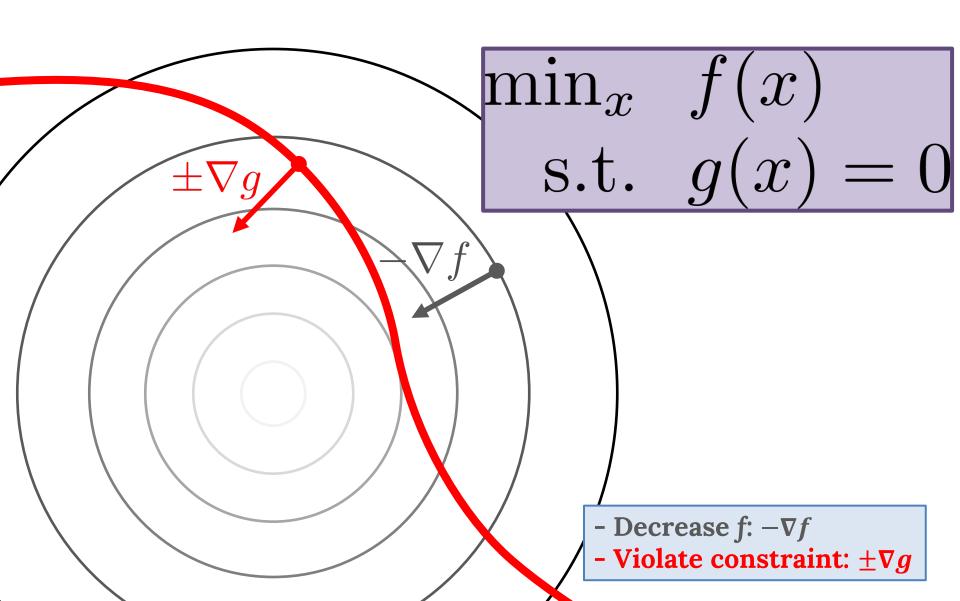
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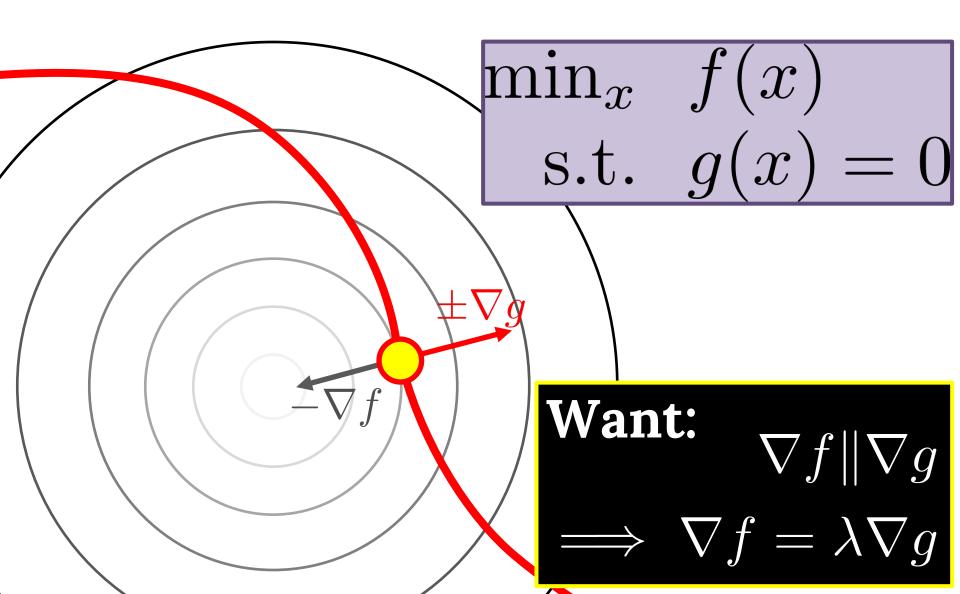
LAGRANGE MULTIPLIERS: IDEA



LAGRANGE MULTIPLIERS: IDEA



LAGRANGE MULTIPLIERS: IDEA



USE OF LAGRANGE MULTIPLIERS

Turns constrained optimization into unconstrained root-finding.

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

$$\min_{x \in \mathbb{R}^n} f(x)$$

$$s.t. g(x) = 0$$

$$\lim_{x \in \mathbb{R}^n} g(x) = 0$$

QUADRATIC WITH LINEAR EQUALITY

$$\min_{x} \quad \frac{1}{2}x^{\top}Ax - b^{\top}x + c$$

s.t.
$$Mx = v$$

(assume A is symmetric and positive definite)

QUADRATIC WITH LINEAR EQUALITY

$$\min_{x} \quad \frac{1}{2}x^{\top}Ax - b^{\top}x + c$$

s.t.
$$Mx = v$$

(assume A is symmetric and positive definite)

$$\begin{pmatrix} A & M^{\top} \\ M & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} b \\ v \end{pmatrix}$$

$$\min_{x \in \mathbb{R}^n} f(x)$$

$$s.t. g(x) = 0$$

$$nonlinear$$

MANY OPTIONS

Reparameterization

Eliminate constraints to reduce to unconstrained case

Newton's method

Approximation: quadratic function with linear constraint

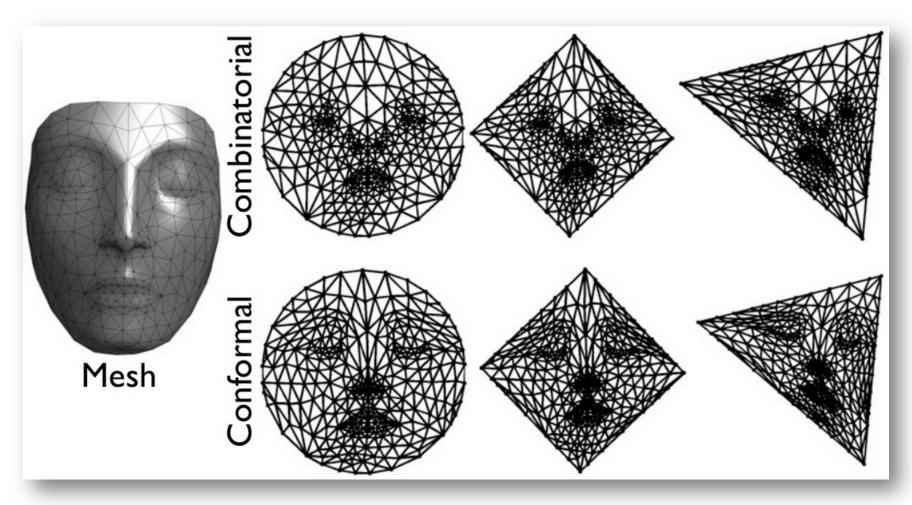
Penalty method

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

EXAMPLE: SYMMETRIC EIGENVECTORS

$$f(x) = x^{\top} Ax \implies \nabla f(x) = 2Ax$$
$$g(x) = ||x||_2^2 \implies \nabla g(x) = 2x$$
$$\implies Ax = \lambda x$$

EXAMPLE: MESH EMBEDDING



G. Peyré, mesh processing course slides

LINEAR SOLVE FOR EMBEDDING

$$x_i \in \mathbb{R}^2$$

$$\min_{\substack{x_1, \dots, x_{|V|} \\ \text{s.t.}}} \sum_{\substack{(i,j) \in E}} w_{ij} ||x_i - x_j||_2^2$$

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

Assumption: w symmetric.

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

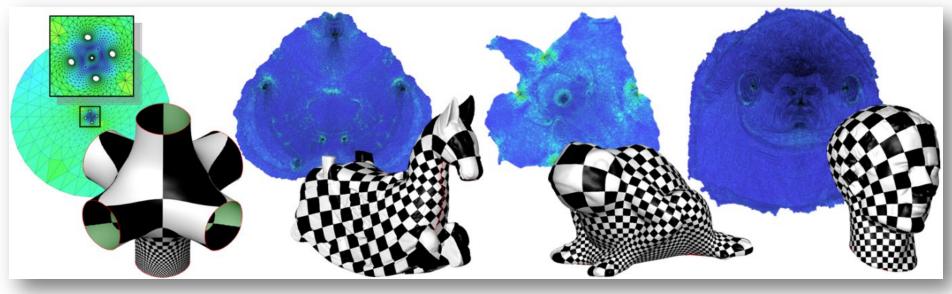
What if $V_0 = \{\}$?

NONTRIVIALITY CONSTRAINT

$$\begin{cases} \min_{x} & ||Ax||_{2} \\ \text{s.t.} & ||x||_{2} = 1 \end{cases} \mapsto A^{\top} Ax = \lambda x$$

Prevents trivial solution $x \equiv 0$.

Extract the smallest eigenvalue.



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

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

BASIC IDEA OF EIGENALGORITHMS

$$A\vec{v} = c_1 A \vec{x}_1 + \dots + c_n A \vec{x}_n$$

$$= c_1 \lambda_1 \vec{x}_1 + \dots + c_n \lambda_n \vec{x}_n \text{ since } A \vec{x}_i = \lambda_i \vec{x}_i$$

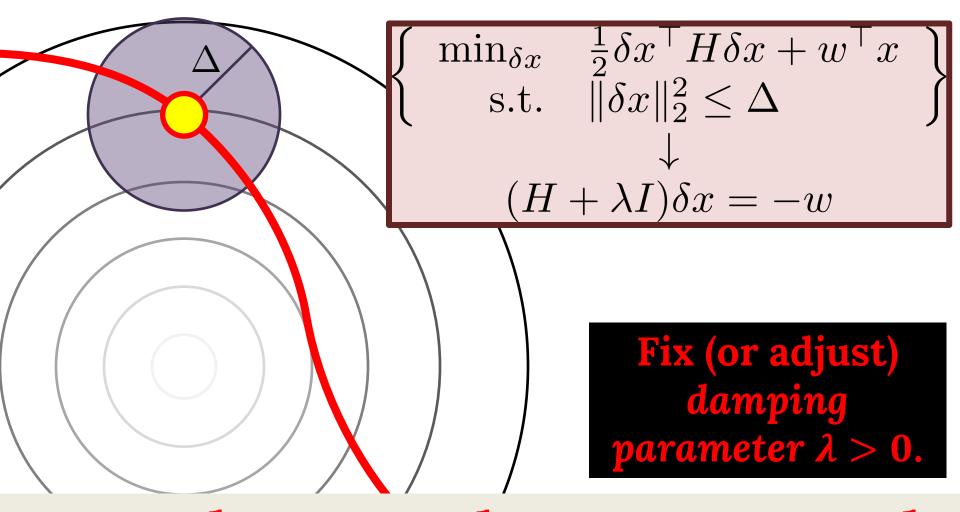
$$= \lambda_1 \left(c_1 \vec{x}_1 + \frac{\lambda_2}{\lambda_1} c_2 \vec{x}_2 + \dots + \frac{\lambda_n}{\lambda_1} c_n \vec{x}_n \right)$$

$$A^2 \vec{v} = \lambda_1^2 \left(c_1 \vec{x}_1 + \left(\frac{\lambda_2}{\lambda_1} \right)^2 c_2 \vec{x}_2 + \dots + \left(\frac{\lambda_n}{\lambda_1} \right)^2 c_n \vec{x}_n \right)$$

$$\vdots$$

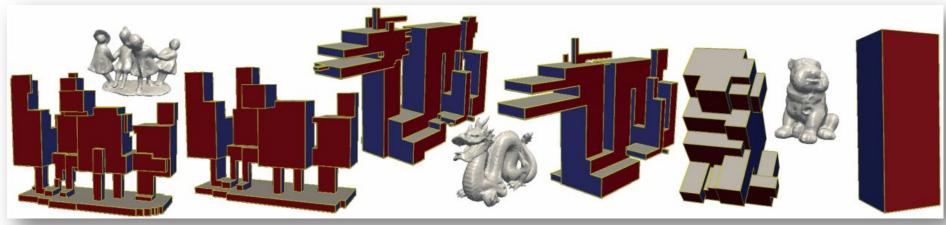
$$A^k \vec{v} = \lambda_1^k \left(c_1 \vec{x}_1 + \left(\frac{\lambda_2}{\lambda_1} \right)^k c_2 \vec{x}_2 + \dots + \left(\frac{\lambda_n}{\lambda_1} \right)^k c_n \vec{x}_n \right).$$

TRUST REGION METHODS



Example: Levenberg-Marquardt

EXAMPLE: POLYCUBE MAPS



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

Align with coordinate axes

$$\min_{X} \sum_{b_i} \mathcal{A}(b_i; X) \| n(b_i; X) \|_1$$

s.t.
$$\sum_{b_i} \mathcal{A}(b_i; X) = \sum_{b_i} \mathcal{A}(b_i; X_0)$$

Note: Final method includes more terms!

Preserve area

Aside:

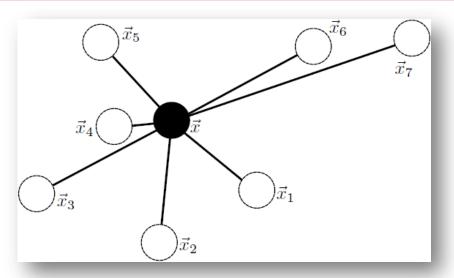
Convex Optimization Tools



Try lightweight options

ITERATIVELY REWEIGHTED LEAST SQUARES

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

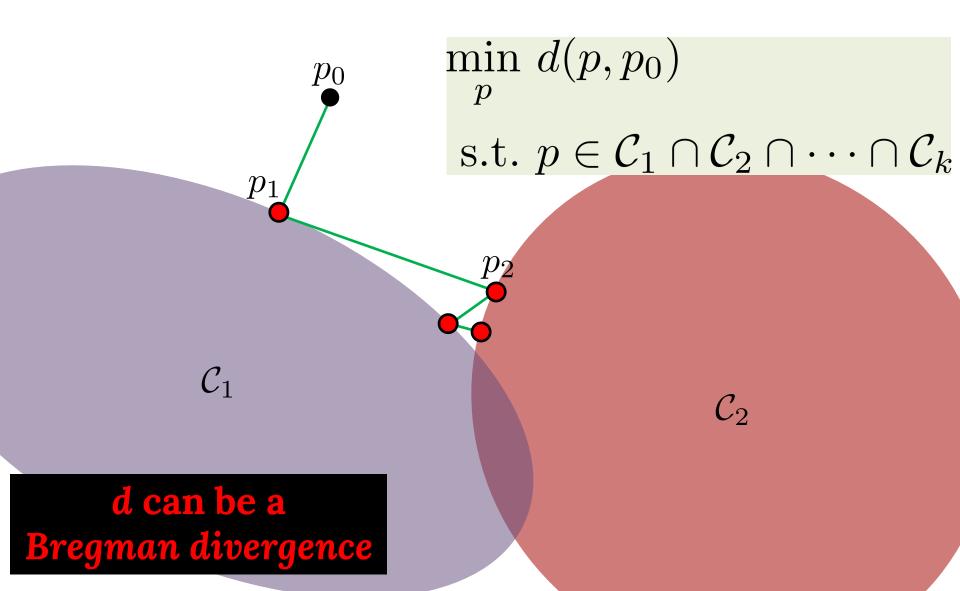


"Geometric median"

$$\min_{x} \sum_{i} \|x - p_i\|_2 \implies \begin{cases} x &\leftarrow \min_{x} \sum_{i} y_i \|x - p_i\|_2^2 \\ y_i &\leftarrow \|x - p_i\|_2^{-1} \end{cases}$$

Repeatedly solve linear systems

ALTERNATING PROJECTION



AUGMENTED LAGRANGIANS

Add constraint to objective

ALTERNATING DIRECTION METHOD OF MULTIPLIERS (ADMM)

(ADMM)

$$\min_{x,z} f(x) + g(z)$$

s.t. $Ax + Bz = c$

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

$$x \leftarrow \arg\min_{x} \Lambda_{\rho}(x, z, \lambda)$$

$$z \leftarrow \arg\min_{z} \Lambda_{\rho}(x, z, \lambda)$$

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

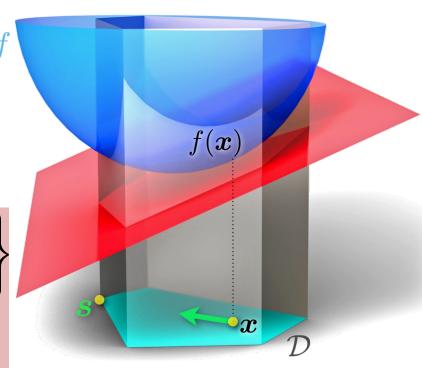
FRANK-WOLFE



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

$$s_k \leftarrow \begin{cases} \arg\min_s & s^{\top} \nabla f(x_k) \\ \text{s.t.} & s \in \mathcal{D} \end{cases}$$
$$\gamma \leftarrow \frac{2}{k+2}$$

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



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

Linearize objective, preserve constraints

ROUGH PLAN

- (intro) Matrices and Eigenvalues
- Linear problems
- Unconstrained optimization
- Equality-constrained optimization
- Variational problems

VARIATIONAL CALCULUS: BIG IDEA

Sometimes your unknowns are not numbers!

Can we use calculus to optimize anyway?

ON THE BOARD

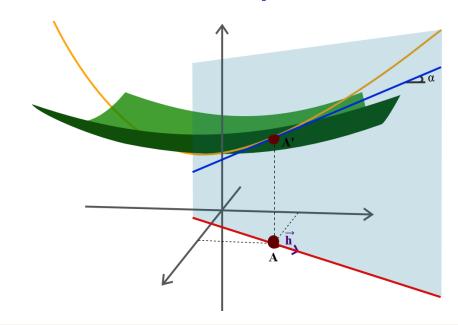
$$\min_{f} \int_{\Omega} \|\vec{v}(x) - \nabla f(x)\|_2^2 d\vec{x}$$

$$\min_{\int_{\Omega} f(x)^2 d\vec{x} = 1} \int_{\Omega} \|\nabla f(x)\|_2^2 d\vec{x}$$

GÂTEAUX DERIVATIVE

$$d\mathcal{F}[u;\psi] := \frac{d}{dh}\mathcal{F}[u+h\psi]|_{h=0}$$

Vanishes for all ψ at a critical point!



Analog of derivative at u in ψ direction