#### IFT 6113 BACKGROUND: LINEAR ALGEBRA AND OPTIMIZATION

#### http://tiny.cc/6113



#### 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.

#### EXAMPLES

#### How to flatten a mesh?



"Mesh Parameterization: Theory and Practice" by Kai Hormann, Bruno Lévy, Alla Sheffer



Credit: Hans-Christian Ebke

#### **EXAMPLES**

How to flatten a mesh?





"Boundary First Flattening" by Rohan Sawhney and Keenan Crane

#### EXAMPLES

#### How to animate a character?



"Linear Subspace Design for Real-Time Shape Deformation" by Yu Wang, Alec Jacobson, Jernej Barbič, Ladislav Kavan

#### EXAMPLES

How to animate a character?

 $\min_{x_i, y_i \in \mathbb{R}^2} f(x_1, y_1, \dots, x_n, y_n)$ s.t.  $x_i - x'_i = 0$  $j \in J$  $y_j - y_i' = 0$ Known positions Triangle Some distortion? smoothness?



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 $h(x) \geq 0$ 



Inequality constraints

#### **EXAMPLES**

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

# EXAMPLES $\begin{array}{l} \max_{x \in \mathbb{R}^{n}} \|Ax\|_{2}^{2} \\ Ax = \lambda x &\leftrightarrow \\ \text{s.t. } \|x\| - 1 = 0 \end{array}$

# **ROUGH PLAN**

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

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How are those matrices special?

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

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

#### How are those matrices special?



#### What is the geometric meaning of those?

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

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

$$& Orthogonal \\ A^{-1} = A^T \qquad Um something?$$

# **INTRO TO INTRO**

#### What is the geometric meaning of those?

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

Non-uniform scaling

$$\begin{pmatrix} \cos(0.4) & -\sin(0.4) & 0\\ \sin(0.4) & \cos(0.4) & 0\\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 3\\ 0 & 1 & 4\\ & & 1 \end{pmatrix}$$
Rotation Translation in 2D\*

#### Eigenvalues and eigenvectors

$$Ax = \lambda x$$
 discrete

or

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

- Geometric transformations
- Linear operators on functions

# **EIGENVECTORS/VALUES**

Geometric meaning?

#### Vectors which only scale



# **MATRIX IS POSITIVE DEFINITE** $A \ge 0$ $\Leftrightarrow$

#### All eigenvalues are nonnegative

Geometric meaning?



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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



# 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<sup>-1</sup> if you can avoid it.

#### SIMPLE EXAMPLE

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



#### **STRUCTURE?**



#### LINEAR SOLVER CONSIDERATIONS

- Never construct A<sup>-1</sup> explicitly (if you can avoid it)
- Added structure helps <u>Sparsity</u>, 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!

Eigen 3.3.5			Q Search
Overview Getting started Chapters	Sparse matrix manipulations         Sparse linear algebra         Manipulating and solving sparse problems involves various modules which are summarized below:		
<ul> <li>Dense many and analy manipulation</li> <li>Dense linear problems and decompositio</li> <li>Sparse linear algebra</li> </ul>			
Sparse matrix manipulations	Module	Header file	Contents
Solving Sparse Linear Systems Matrix-free solvers	SparseCore	<pre>#include <eigen sparsecore=""></eigen></pre>	SparseMatrix and SparseVector classes, matrix assembly, basic sparse linear algebra (including sparse triangular solvers)
Quick reference guide for sparse matr	SparseCholesky	<pre>#include <eigen sparsecholesky=""></eigen></pre>	Direct sparse LLT and LDLT Cholesky factorization to solve sparse self-adjoint positive definite problems
Geometry	SparseLU	<pre>#include<eigen sparselu=""></eigen></pre>	Sparse LU factorization to solve general square sparse systems
Extending/Customizing Eigen     General tonics	SparseQR	<pre>#include<eigen sparseqr=""></eigen></pre>	Sparse QR factorization for solving sparse linear least-squares problems
Table of contents	IterativeLinearSolvers	<pre>#include <eigen iterativelinearsolvers=""></eigen></pre>	Iterative solvers to solve large general linear square problems (including self-adjoint positive definite problems)
	Sparse	<pre>#include <eigen sparse=""></eigen></pre>	Includes all the above modules
	Sparse matrix format In many applications (e.g., finite element methods) it is common to deal with very large matrices where only a few coefficients are different from zero. In such cases, memory consumption can be reduced and performance increased by using a specialized		
↓ Sparse matrix format ↓ First example	representation storing only the nonzero coefficients. Such a matrix is called a sparse matrix.		
<ul> <li>Une SparseMatrix class</li> <li>Uniting a sparse matrix</li> <li>Supported operators and functions</li> <li>Basic operations</li> <li>Matrix products</li> <li>Block operations</li> </ul>	The SparseMatrix class		
	The class SparseMatrix is the main sparse matrix representation of Eigen's sparse module; it offers high performance and low memory usage. It implements a more versatile variant of the widely-used Compressed Column (or Row) Storage scheme. It consists of four compact arrays:		
Triangular and selfadjoint views			

#### https://eigen.tuxfamily.org/dox/group\_\_TutorialSparse.html

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#### UNCONSTRAINED OPTIMIZATION



Trivial when f(x) is linear

Easy when f(x) is quadratic

Hard in case of generic non-linear.



$$f(x, y) = 3x^2 - y$$
$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (6x, -1)$$

Geometric meaning?





Gradient

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

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



Gradient

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



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





**Critical point** 



https://en.wikipedia.org/wiki/Convex\_function

## **CONVEX FUNCTIONS** $H(x) \ge 0$



https://en.wikipedia.org/wiki/Convex\_function

#### SPECIAL CASE: LEAST-SQUARES

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

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

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

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



#### **BASIC ALGORITHMS**



#### Gradient descent

## **BASIC ALGORITHMS**

$$egin{aligned} &\lambda_0 = 0, \lambda_s = rac{1}{2}(1 + \sqrt{1 + 4\lambda_{s-1}^2}), \gamma_s = rac{1 - \lambda_2}{\lambda_{s+1}} \ &y_{s+1} = x_s - rac{1}{eta} 
abla f(x_s) \ &x_{s+1} = (1 - \gamma_s) y_{s+1} + \gamma_s y_s \end{aligned}$$

Quadratic convergence on convex problems! (Nesterov 1983)

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

## Accelerated gradient descent

#### **BASIC ALGORITHMS**

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



#### Newton's Method



- (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.



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

е

e

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:  $\int \|\nabla f\|_2$ ???: Early stopping Regularization

## **SOME TRICKS**





Original

Blurred

## Multiscale/graduated optimization

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#### LAGRANGE MULTIPLIERS: IDEA



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#### USE OF LAGRANGE MULTIPLIERS

#### Turns constrained optimization into unconstrained root-finding.

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



#### QUADRATIC WITH LINEAR EQUALITY

$$\min_{x} \quad \frac{1}{2}x^{\top}Ax - b^{\top}x + c \\ \text{s.t.} \quad Mx = v$$

(assume A is symmetric and positive definite)

#### QUADRATIC WITH LINEAR EQUALITY




## 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

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

#### EXAMPLE: MESH EMBEDDING



G. Peyré, mesh processing course slides

#### LINEAR SOLVE FOR EMBEDDING

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

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

- $w_{ij} \equiv 1$ : Tutte embedding
- *w<sub>ij</sub>* from mesh: Harmonic embedding

#### Assumption: w symmetric.

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

What if 
$$V_0 = \{\}$$
?

#### **NONTRIVIALITY CONSTRAINT**

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

#### **Prevents** trivial solution $x \equiv 0$ .

#### Extract the smallest eigenvalue.



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

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

#### BASIC IDEA OF EIGENALGORITHMS

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

#### **TRUST REGION METHODS**



#### **Example: Levenberg-Marquardt**

#### **EXAMPLE: POLYCUBE MAPS**



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

$$\begin{aligned} & \underset{X \in \mathcal{A}(b_i; X) \\ \text{min}_X \sum_{b_i} & \mathcal{A}(b_i; X) \| n(b_i; X) \|_1 \\ & \text{s.t.} & \sum_{b_i} \mathcal{A}(b_i; X) = \sum_{b_i} \mathcal{A}(b_i; X_0) \end{aligned}$$

Note: Final method includes more terms!

#### **Preserve area**

#### Aside: Convex Optimization Tools



## **Try lightweight options**

#### ITERATIVELY REWEIGHTED LEAST SQUARES



### **Repeatedly solve linear systems**

#### **ALTERNATING PROJECTION**

p

 $p_2$ 

 $p_0$ 

 $p_1$ 

min  $d(p, p_0)$ 

s.t.  $p \in \mathcal{C}_1 \cap \mathcal{C}_2 \cap \cdots \cap \mathcal{C}_k$ 

 $\mathcal{C}_2$ 



 $\mathcal{C}_1$ 

#### **AUGMENTED LAGRANGIANS**

$$\begin{array}{ll} \min_{x} & f(x) \\ \text{s.t.} & g(x) = 0 \\ & \downarrow \\ \min_{x} & f(x) + \frac{\rho}{2} \|g(x)\|_{2}^{2} \end{array} \xrightarrow{\text{Does nothing when}} \\ \text{s.t.} & g(x) = 0 \end{array}$$

## Add constraint to objective

#### ALTERNATING DIRECTION METHOD OF MULTIPLIERS (ADMM) $\min_{x,z} f(x) + g(z)$ s.t. Ax + Bz = c

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

$$\begin{aligned} x \leftarrow \arg \min_{x} \Lambda_{\rho}(x, z, \lambda) \\ z \leftarrow \arg \min_{z} \Lambda_{\rho}(x, z, \lambda) \\ \lambda \leftarrow \lambda + \rho(Ax + Bz - c) \end{aligned}$$

https://web.stanford.edu/~boyd/papers/pdf/admm\_slides.pdf

#### **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

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#### 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  $\psi$  at a critical point!



#### Analog of derivative at u in $\psi$ direction