Linear and Quadratic Programming (with CGAL)

Bernd Gärtner, Algorithms Lab

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Linear Programming (LP)

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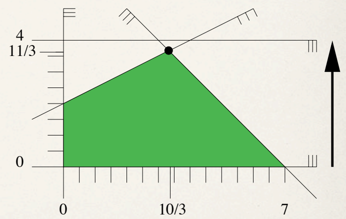

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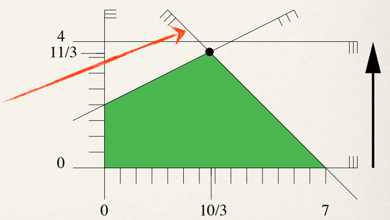

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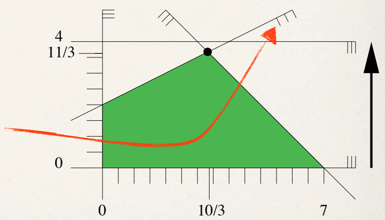

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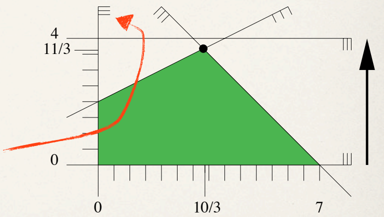

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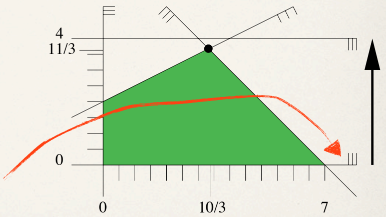

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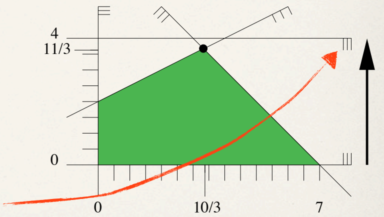

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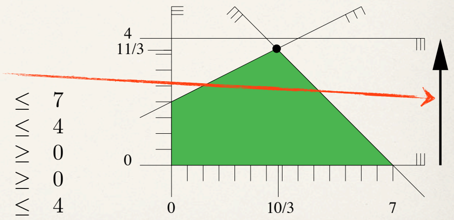

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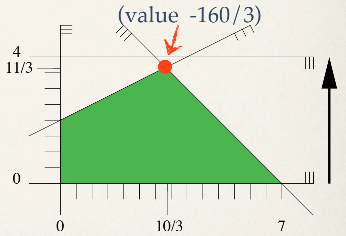
Optimal solution (value -160/3)

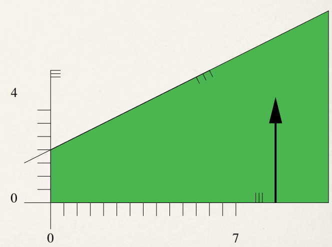


Linear Programming

- **Problem:** Minimize a linear function in n variables subject to m linear (in)equality constraints!
- **Unbounded linear programs:**

$$\begin{array}{lrcl} \text{minimize} & -32y+64 & & \\ \text{subject to} & x+y & \leq & 7 \\ & -x+2y & \leq & 4 \\ & x & \geq & 0 \\ & y & \geq & 0 \\ & y & \leq & 4 \end{array}$$

(The constraints $x+y \leq 7$ and $y \leq 4$ are struck through.)



Linear Programming

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- **Infeasible linear programs:**

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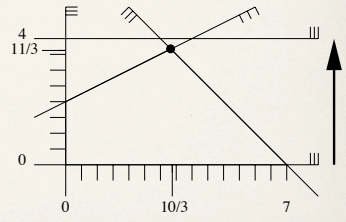

Linear Programming ... in CGAL

- **General form of LP in CGAL:**

$$\begin{array}{ll} \text{minimize} & c^T x + c_0 \\ \text{subject to} & Ax \gtreqless b \\ & l \leq x \leq u \end{array}$$

$$(x, c, l, u \in \mathbb{R}^n, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m, \quad c_0 \in \mathbb{R})$$

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≤, =, or ≥ (individually for each constraint)

variables

$$(x, c, l, u \in \mathbb{R}^n, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m, \quad c_0 \in \mathbb{R})$$

objective function

lower and upper bounds

constraint matrix

right-hand side

shift

Linear Programming ... in CGAL

$$\begin{array}{lrcl} \text{minimize} & -32y + 64 & & \\ \text{subject to} & x + y & \leq & 7 \\ & -x + 2y & \leq & 4 \\ & x & \geq & 0 \\ & y & \geq & 0 \\ & y & \leq & 4 \end{array}$$

- **Preamble:** Choice of input type and exact internal number type

Gnu Multi-precision Library (GMP)

CGAL

```
#include <iostream>
#include <cassert>
#include <CGAL/basic.h>
#include <CGAL/QP_models.h>
#include <CGAL/QP_functions.h>

// choose exact integral type
#ifdef CGAL_USE_GMP
#include <CGAL/Gmpz.h>
typedef CGAL::Gmpz ET;
#else
#include <CGAL/MP_Float.h>
typedef CGAL::MP_Float ET;
#endif

// program and solution types
typedef CGAL::Quadratic_program<int> Program;
typedef CGAL::Quadratic_program_solution<ET> Solution;
```

input type

exact internal type

for linear *and* quadratic programs

GMP used internally

Linear Programming ... in CGAL

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- **Setup:** Enter the program data

```
int main() {
  // by default, we have a nonnegative LP with Ax <= b
  Program lp (CGAL::SMALLER, true, 0, false, 0);

  // now set the non-default entries
  const int X = 0;
  const int Y = 1;
  lp.set_a(X, 0,  1); lp.set_a(Y, 0, 1); lp.set_b(0, 7);  //  x + y  <= 7
  lp.set_a(X, 1, -1); lp.set_a(Y, 1, 2); lp.set_b(1, 4);  // -x + 2y <= 4
  lp.set_u(Y, true, 4);                                   //        y <= 4
  lp.set_c(Y, -32);                                       // -32y
  lp.set_c0(64);                                          // +64
```

$l =$ (0,0,..., 0)

$u = (\infty, \infty, \ldots, \infty)$

last argument: value

variable index (0,1,...)

constraint index (0,1,...)

Linear Programming ... in CGAL

- **Solve:** Call the linear programming solver and output solution

```
  // solve the program, using ET as the exact type
  Solution s = CGAL::solve_linear_program(lp, ET());
  assert (s.solves_linear_program(lp));

  // output solution
  std::cout << s;
  return 0;
}
```

independent verification

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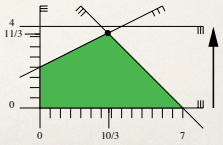
}
```

independent verification

- **Output:**

```
status:               OPTIMAL
objective value:      -160/3
variable values:
  0:  10/3
  1:  11/3
```



Linear Programming Application I: Cancer Therapy

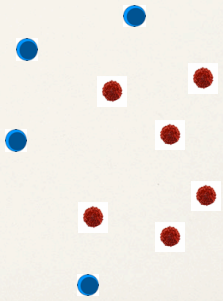
- **Given:** locations of cancer cells (red)

Linear Programming Application I: Cancer Therapy

- **Given:** locations of cancer cells (red) and healthy cells (blue)

Linear Programming Application I: Cancer Therapy

- **Given:** locations of cancer cells (red) and healthy cells (blue)
- **Wanted:** center and radius of exposure so that all cancer cells are killed and all healthy cells are unaffected.



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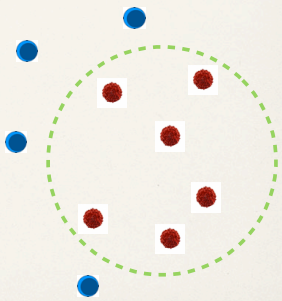
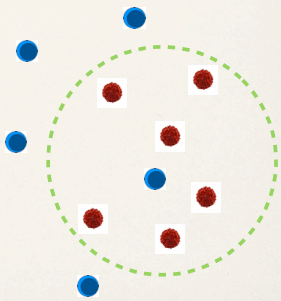
- This may be possible...



Linear Programming Application I: Cancer Therapy

- **Given:** locations of cancer cells (red) and healthy cells (blue)
- **Wanted:** center and radius of exposure so that all cancer cells are killed and all healthy cells are unaffected.
- This may be possible... or not.



Linear Programming
Application I: Cancer Therapy

- **The geometric problem:** Given two finite sets R and B in the plane, does there exist a disk that contains R and is disjoint from B?

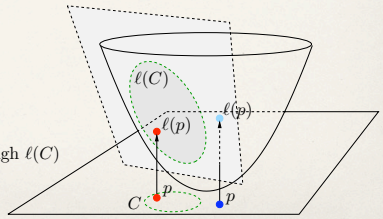
Linear Programming
Application I: Cancer Therapy

- **The geometric problem:** Given two finite sets R and B in the plane, does there exist a disk that contains R and is disjoint from B?
- Apply *lifting map* $\ell : (x, y) \mapsto (x, y, x^2 + y^2)$

p { inside / on / outside } C

$\Updownarrow$

$\ell(p)$ { below / on / above } the plane through $\ell(C)$



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plane: $z = \alpha x + \beta y + \gamma$

Linear Programming
Application I: Cancer Therapy

- **The geometric problem (lifted space):** Given the lifted sets R' and B' in space, is there a plane that has R' below/on it and B' above?
- This is linear programming!
- Find $\alpha, \beta, \gamma, \delta > 0$ such that...

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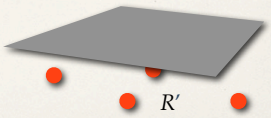

$$x^2 + y^2 \leq \alpha x + \beta y + \gamma, \quad (x, y) \in R$$

Linear Programming Application I: Cancer Therapy

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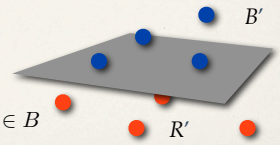

$$x^2 + y^2 \geq \alpha x + \beta y + \gamma + \delta, \quad (x, y) \in B$$
$$x^2 + y^2 \leq \alpha x + \beta y + \gamma, \quad (x, y) \in R$$

Linear Programming Application I: Cancer Therapy

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- This is linear programming!
- Find $\alpha, \beta, \gamma, \delta > 0$ such that...

plane: $z = \alpha x + \beta y + \gamma$

4 variables
|B|+|R| constraints

maximize δ

subject to

$$x^2 + y^2 \geq \alpha x + \beta y + \gamma + \delta, \quad (x, y) \in B$$
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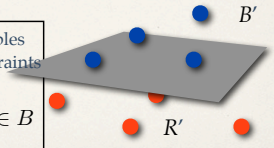

Linear Programming Application I: Cancer Therapy

- **Fact:** Exposure is possible if and only if the following linear program has positive value.

maximize δ

subject to

$$x^2 + y^2 \geq \alpha x + \beta y + \gamma + \delta, \quad (x, y) \in B$$
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- **Reconstructing the exposure from an optimal solution** ($\alpha, \beta, \gamma, \delta$):

$$= \{(x, y) : x^2 + y^2 = \alpha x + \beta y + \gamma\}$$

Linear Programming Application I: Cancer Therapy

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$$= \{(x, y) : (x - \frac{\alpha}{2})^2 + (y - \frac{\beta}{2})^2 = \gamma + \frac{\alpha^2}{4} + \frac{\beta^2}{4}\}$$

Linear Programming Application I: Cancer Therapy

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maximize δ

subject to

$$x^2 + y^2 \geq \alpha x + \beta y + \gamma + \delta, \quad (x,y) \in B$$
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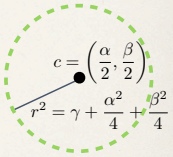


- **Reconstructing the exposure from an optimal solution** (α, β, γ, δ):

$$= \{(x,y) : x^2 + y^2 = \alpha x + \beta y + \gamma\}$$
$$= \{(x,y) : (x - \frac{\alpha}{2})^2 + (y - \frac{\beta}{2})^2 = \gamma + \frac{\alpha^2}{4} + \frac{\beta^2}{4}\}$$

Linear Programming Application I: Cancer Therapy

- **Implementation in CGAL:**

minimize $-\delta$

subject to

$$x^2 + y^2 \geq \alpha x + \beta y + \gamma + \delta, \quad (x,y) \in B$$
$$x^2 + y^2 \leq \alpha x + \beta y + \gamma, \quad (x,y) \in R$$
$$\delta \leq 1$$

Avoids unbounded program

maximize $c^T x \rightarrow$ minimize $-c^T x$ and negate resulting value

Linear Programming Application I: Cancer Therapy

- **Implementation in CGAL: Setup and Solve** (Preamble as before)

```
int main() {
  // by default, we have an LP with Ax <= b and no bounds for
  // the four variables alpha, beta, gamma, delta
  Program lp (CGAL::SMALLER, false, 0, false, 0);
  const int alpha = 0;
  const int beta  = 1;
  const int gamma = 2;
  const int delta = 3;

  // number of red and blue points
  int m; std::cin >> m;
  int n; std::cin >> n;

  // read the red points (cancer cells)
  for (int i=0; i<m; ++i) {
    int x; std::cin >> x;
    int y; std::cin >> y;
    // set up <= constraint for point inside/on circle:
    //   -alpha x - beta y - gamma <= -x^2 - y^2
    lp.set_a (alpha, i, -x);
    lp.set_a (beta,  i, -y);
    lp.set_a (gamma, i, -1);
    lp.set_b (       i, -x*x - y*y);
  }
```

```
  // read the blue points (healthy cells)
  for (int j=0; j<n; ++j) {
    int x; std::cin >> x;
    int y; std::cin >> y;
    // set up <= constraint for point outside circle:
    //   alpha x + beta y + gamma + delta <= x^2 + y^2
    lp.set_a (alpha, m+j, x);
    lp.set_a (beta,  m+j, y);
    lp.set_a (gamma, m+j, 1);
    lp.set_a (delta, m+j, 1);
    lp.set_b (       m+j, x*x + y*y);
  }

  // objective function: -delta (the solver minimizes)
  lp.set_c(delta, -1);

  // enforce a bounded problem:
  lp.set_u (delta, true, 1);

  // solve the program, using ET as the exact type
  Solution s = CGAL::solve_linear_program(lp, ET());
  assert (s.solves_linear_program(lp));
```


Linear Programming Application I: Cancer Therapy

- **Implementation in CGAL: Output**

negate resulting value!

```
  // output exposure center and radius, if they exist
  if (s.is_optimal() && (s.objective_value() < 0)) {
    // *opt := alpha, *(opt+1) := beta, *(opt+2) := gamma
    CGAL::Quadratic_program_solution<ET>::Variable_value_iterator
      opt = s.variable_values_begin();
    CGAL::Quotient<ET> alpha = *opt;
    CGAL::Quotient<ET> beta = *(opt+1);
    CGAL::Quotient<ET> gamma = *(opt+2);
    std::cout << "There is a valid exposure:\n";
    std::cout << " Center = ("         // (alpha/2, beta/2)
         << alpha/2 << ", " <<  beta/2
         << ")\n";
    std::cout << " Squared Radius = " // gamma + alpha^2/4 + beta^2/4
         << gamma + alpha*alpha/4 + beta*beta/4 << "\n";
  } else
    std::cout << "There is no valid exposure.";
  std::cout << "\n";
  return 0;
}
```


Linear Programming Application I: Cancer Therapy

- **Implementation in CGAL: Output**

negate resulting value!

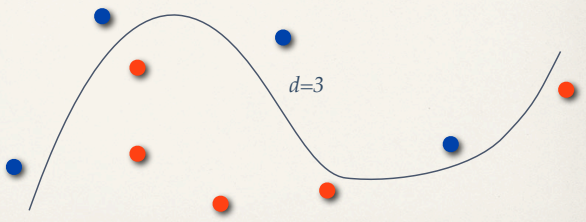
"Pointer" to first variable of optimal solution

The quotient `*(opt+i)` is the value of the variable x_i in the optimal solution

```
  // output exposure center and radius, if they exist
  if (s.is_optimal() && (s.objective_value() < 0)) {
    // *opt := alpha, *(opt+1) := beta, *(opt+2) := gamma
    CGAL::Quadratic_program_solution<ET>::Variable_value_iterator
      opt = s.variable_values_begin();
    CGAL::Quotient<ET> alpha = *opt;
    CGAL::Quotient<ET> beta = *(opt+1);
    CGAL::Quotient<ET> gamma = *(opt+2);
    std::cout << "There is a valid exposure:\n";
    std::cout << " Center = ("         // (alpha/2, beta/2)
         << alpha/2 << ", " <<  beta/2
         << ")\n";
    std::cout << " Squared Radius = " // gamma + alpha^2/4 + beta^2/4
         << gamma + alpha*alpha/4 + beta*beta/4 << "\n";
  } else
    std::cout << "There is no valid exposure.";
  std::cout << "\n";
  return 0;
}
```


Linear Programming Beyond Cancer Therapy

- Given a set of R of red and a set B of blue points, can they be separated by the zero set of a polynomial of degree *d*?



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- Linear programming formulation: find *a,b,c,d,e,f,g,h,i,j* such that

$$ax^3 + bx^2y + cxy^2 + dy^3 + ex^2 + fxy + gy^2 + hx + iy + j \leq 0, \quad (x,y) \in B$$
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- This is linear separability in 8-dimensional space, under the generalized lifting map $(x,y) \to (x^3, x^2y, xy^2, y^3, x^2, xy, y^2, x, y)$

Linear Programming Further Applications

- Linear-fractional programming LFP:

$$\begin{array}{lrcl} \text{minimize} & & \frac{c^Tx+d}{e^Tx+f} & \\ \text{subject to} & Ax & \leqslant \geqslant & b \\ & e^Tx+f & > & 0 \end{array}$$

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x feasible with value t

$y = \frac{x}{e^Tx+f}, z = \frac{1}{e^Tx+f}$ feasible with value t

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$x = \frac{y}{z}$ feasible with value t

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$z = 0$: can be handled if LFP is feasible

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- Linear programming relaxations for hard combinatorial problems

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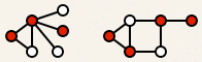
- **Vertex Cover:** Given a graph G=(V,E), find a smallest subset of vertices (a vertex cover) such that every edge is incident to one vertex of the cover.



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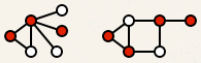

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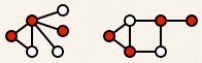

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← not an LP!

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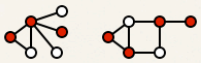

- Let $x^*_1, x^*_2, \ldots, x^*_n$ be an optimal solution of the *LP relaxation*

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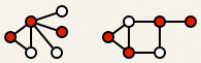

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- **Theorem:** C = {i: $x^*_i \geq 1/2$} is a vertex cover of size at most 2 opt.

Wednesday, November 21, 2012

Linear vs. Integer Programming

- Often, applications lead to linear programs with the additional requirement of *integral solutions* (e.g. vertex cover)

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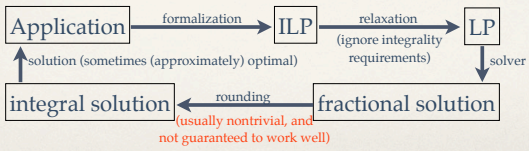

Wednesday, November 21, 2012

Quadratic Programming (QP)

- **Problem:** Minimize a convex quadratic function in *n* variables subject to *m* linear (in)equality constraints!

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- **Example** (n=2, m=5):

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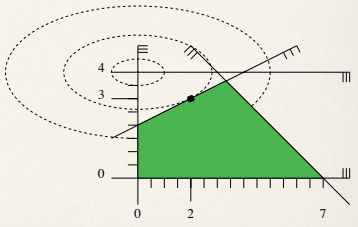

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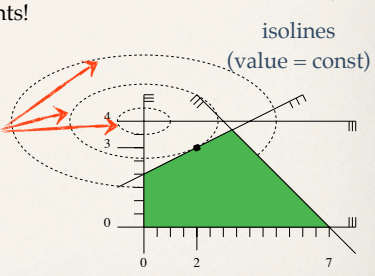

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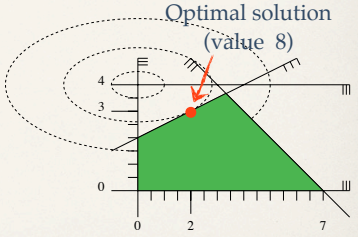

Quadratic Programming ... in CGAL

- **General form of QP in CGAL:**

$$\begin{array}{ll} \text{minimize} & x^T Dx + c^T x + c_0 \\ \text{subject to} & Ax \gtreqless b \\ & l \leq x \leq u \end{array}$$

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- **Relax:** In the applications, we know from theory that D is "good"

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- **Code:** at the very end of this presentation...

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- After the training phase, the system is supposed to decide on its own which letter it sees.

Quadratic Programming: Support Vector Machines

- Solution: map training letters to points in some high-dimensional space, with label 'A' (blue) or 'B' (red), based e.g. on a pixel-based representation

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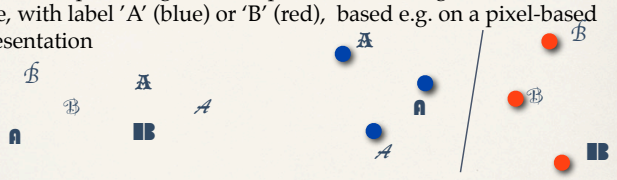

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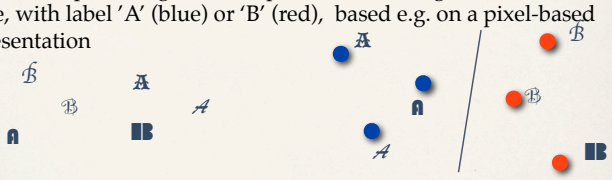

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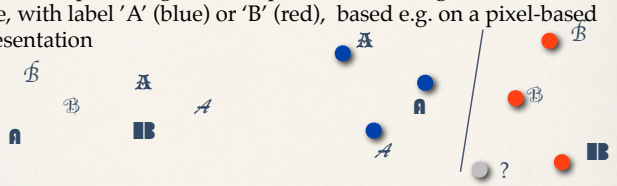

- Separate the 'A's from the 'B's by a simple shape, for example the *maximum-margin hyperplane* (separating hyperplane of maximum distance to any point). **This is a quadratic program!**
- Classify an unknown letter according to this hyperplane (= 'B')

Quadratic Programming: Support Vector Machines

- Other separating shapes (e.g. spheres as in the cancer therapy application, or zero sets of polynomials) can make sense
- Through lifting, we can often reduce the problem for a given separating shape to the problem of finding the maximum-margin separating hyperplane in some higher (sometimes even infinite-dimensional space). In the end, we just need to solve a quadratic program!

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- In the world of support vector machines, the problem of selecting the appropriate separating shape is called *kernel design*.

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- **Risk-tolerant strategy:** Minimize the risk under a given lower bound for the expected return!

Quadratic Programming Application: Low-Risk Investment

- Possible **investments:**
  - $1,2,\ldots,n$ (e.g. 1 = Swatch shares, 2 = Credit Suisse shares,...)
- **Investment Characteristics** (not at all easy to know/estimate)**:**
  - R_i : return rate of investment i (assumed to be a random variable)
  - r_i : expected return rate of investment i, $E[R_i]$
  - v_i : variance ("risk") of R_i, $\mathrm{Var}[R_i] := E[(R_i - E[R_i])^2]$
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$v_{ii} = v_i$

Quadratic Programming Application: Low-Risk Investment

- **Example:** $n=2$

	r_i
Swatch shares	10% (0.1)
Credit Suisse shares	51% (0.51)

v_{ij}	Swatch shares	Credit Suisse shares
Swatch shares	0.09	-0.05
Credit Suisse shares	-0.05	0.25

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Negative correlation: if CS does worse than expected, Swatch will probably do better, and vice versa

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Read as: standard deviation of return rate is $\sqrt{0.25} = 0.5$ (actual return rate could easily be off by 0.5)

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- **Investment strategy:**

$$(x_1, x_2, \ldots, x_n), \quad \sum_{i=1}^{n} x_i = 1, \quad x_i \geq 0 \forall i$$

Meaning: An x_i fraction of your money goes into investment *i*

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- **Expected return rate of this strategy:**

$$E[\sum_{i=1}^{n} x_i R_i] = \sum_{i=1}^{n} x_i E[R_i] = \sum_{i=1}^{n} r_i x_i$$

Quadratic Programming Application: Low-Risk Investment

- **Investment strategy:**

$$(x_1, x_2, \ldots, x_n), \quad \sum_{i=1}^{n} x_i = 1, \quad x_i \geq 0 \forall i$$

Meaning: An x_i fraction of your money goes into investment *i*

- **Expected return rate of this strategy:**

$$E[\sum_{i=1}^{n} x_i R_i] = \sum_{i=1}^{n} x_i E[R_i] = \sum_{i=1}^{n} r_i x_i$$

- **Example:** half the money in Swatch shares, half in Credit Suisse shares; expected return rate is $\frac{1}{2} \cdot 0.1 + \frac{1}{2} \cdot 0.51 = 0.305 = 30.5\%$

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- **Risk of this strategy:**

Straightforward calculations

$$\mathrm{Var}[\sum_{i=1}^{n} x_i R_i] = \sum_{i=1}^{n} \sum_{j=1}^{n} v_{ij} x_i x_j = x^T D x$$

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less than each individual risk!

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Wednesday, November 21, 2012

Quadratic Programming Application: Low-Risk Investment

- **The risk-tolerant case:** Find the investment strategy with lowest risk that guarantees expected return rate at least ρ!

$$\begin{aligned} \text{minimize} \quad & \sum_{i=1}^{n}\sum_{j=1}^{n} v_{ij} x_i x_j \leftarrow \text{risk} \\ \text{subject to} \quad & \sum_{i=1}^{n} r_i x_i \geq \rho \leftarrow \text{expected return rate} \\ & \sum_{i=1}^{n} x_i = 1 \leftarrow \text{strategy} \\ & x_i \geq 0, \quad i = 1, \ldots, n \end{aligned}$$

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Fact: the covariance matrix is positive semidefinite, so this is indeed a convex QP.

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- **Example:** $\rho = 0.4$: 26.8% Swatch, 73.2% Credit Suisse; risk $= 0.121$

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Low-Risk Investment Example ... in CGAL

- **Preamble:** This time, it's floating-point input...

Gnu Multi-precision Library (GMP)

CGAL

```
#include <iostream>
#include <cassert>
#include <CGAL/basic.h>
#include <CGAL/QP_models.h>
#include <CGAL/QP_functions.h>

// choose exact floating-point type
#ifdef CGAL_USE_GMP
#include <CGAL/Gmpzf.h>
typedef CGAL::Gmpzf ET;
#else
#include <CGAL/MP_Float.h>
typedef CGAL::MP_Float ET;
#endif

// program and solution types
typedef CGAL::Quadratic_program<double> Program;
typedef CGAL::Quadratic_program_solution<ET> Solution;
```

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Low-Risk Investment Example ... in CGAL

- **Input:** Desired expected return

```
int main() {
  // read minimum expected return rate
  std::cout << "What is your desired expected return rate? ";
  double rho; std::cin >> rho;
```

for example, 0.4 = 40%

Low-Risk Investment Example ... in CGAL

- **Setup:** Make sure to enter matrix *2D* (customary in QP solvers)!

```
  // by default, we have a nonnegative QP with Ax >= b
  Program qp (CGAL::LARGER, true, 0, false, 0);

  // now set the non-default entries:
  const int sw = 0;
  const int cs = 1;

  // constraint on expected return: 0.1 sw + 0.51 cs >= rho
  qp.set_a(sw, 0, 0.1);
  qp.set_a(cs, 0, 0.51);
  qp.set_b(    0, rho);

  // strategy constraint: sw + cs = 1
  qp.set_a(sw, 1, 1);
  qp.set_a(cs, 1, 1);
  qp.set_b(    1, 1);
  qp.set_r(    1, CGAL::EQUAL); // override default >=

  // objective function: 0.09 sw^2 - 0.1 sw cs - 0.1 cs sw + 0.25 cs^2
  // we need to specify the entries of the symmetric matrix 2D, on and below the diagonal
  qp.set_d(sw, sw,  0.18); //  0.09 sw^2
  qp.set_d(cs, sw, -0.10); // -0.05 cs sw
  qp.set_d(cs, cs,  0.5);  //  0.25 cs^2
```

$j \leq i$ in `set_d (i, j)`

Low-Risk Investment Example ... in CGAL

- **Solve:** ...as nonnegative quadratic program (a little faster)

```
  // solve the program, using ET as the exact type
  Solution s = CGAL::solve_nonnegative_quadratic_program(qp, ET());
  assert (s.solves_quadratic_program(qp));
```

independent verification

Low-Risk Investment Example ... in CGAL

- **Output:** query programming status; if feasible, output strategy / risk

```
  // output
  if (s.status() == CGAL::QP_INFEASIBLE) {
    std::cout << "Expected return rate " << rho << " cannot be achieved.\n";
  } else {
    assert (s.status() == CGAL::QP_OPTIMAL);
    Solution::Variable_value_iterator opt =
      s.variable_values_begin();
    CGAL::Quotient<ET> sw_fraction = *opt;
    CGAL::Quotient<ET> cs_fraction = *(opt+1);
    std::cout << "Minimum risk investment strategy:\n";
    std::cout << 100.0*CGAL::to_double(sw_fraction)
         << "%" << " into Swatch\n";
    std::cout << 100.0*CGAL::to_double(cs_fraction)
         << "%" << " into Credit Suisse\n";
    std::cout << "Risk = " << CGAL::to_double(s.objective_value()) << "\n";
  }
  return 0;
}
```


Sources and Further Reading

- **LP/QP Solver:** Online manual at **`www.cgal.org`**: Online Manual → Combinatorial Algorithms → Linear and Quadratic Programming Solver
- **Cancer Therapy:** J. O'Rourke, S. Kosaraju, and N. Megiddo: Computing Circular Separabiliy, *Discrete & Computational Geometry* 1:105-113 (1986)
- **Support Vector Machines:** B. Schölkopf, A. J. Smola: *Learning with Kernels*, MIT Press, 2002
- **Low-Risk Investment:** H. Markowitz: Portfolio Selection, *Journal of Finance* 7(1): 77-91 (1952)