Support Vector Machines Meet Goldfarb Cubes

Bernd Gärtner, IPAM Conference "Quo Vadis Hirsch Conjecture?"

January 19, 2011

Disproving the Hirsch Conjecture of Machine Learning

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Outline

- Introduction to Support Vector Machines, and their interpretation as parametric *quadratic* programs
- Statement of the main result: disproof of a conjecture by Hastie et al. concerning the solution path complexity of support vector machines
- Parametric *linear* programs, the shadow vertex pivot rule, and the Goldfarb cubes
- Putting it together: constructing exponentially long solution paths for support vector machines, using Goldfarb cubes (sketch)

Support Vector Machines (SVM)

- Suppose an optical character recognition needs to distinguish between the letters ‘A’ and ‘B’

Support Vector Machines

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- Training phase: the system gets to see letters ‘A’ and ‘B’ **plus** the information whether it’s an ‘A’ or a ‘B’

Support Vector Machines

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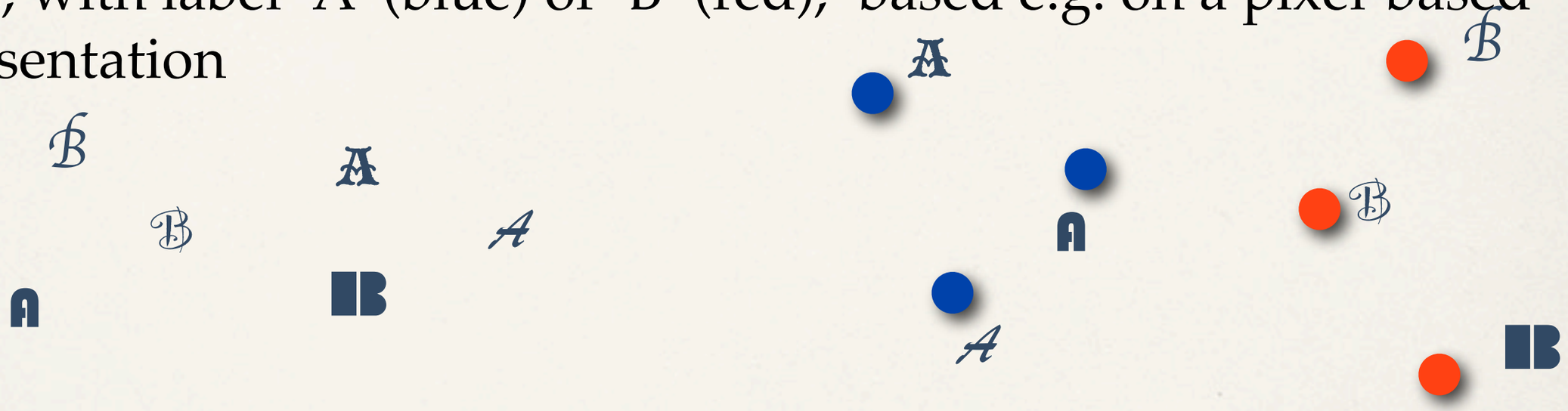
- Training phase: the system gets to see letters ‘A’ and ‘B’ **plus** the information whether it’s an ‘A’ or a ‘B’

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

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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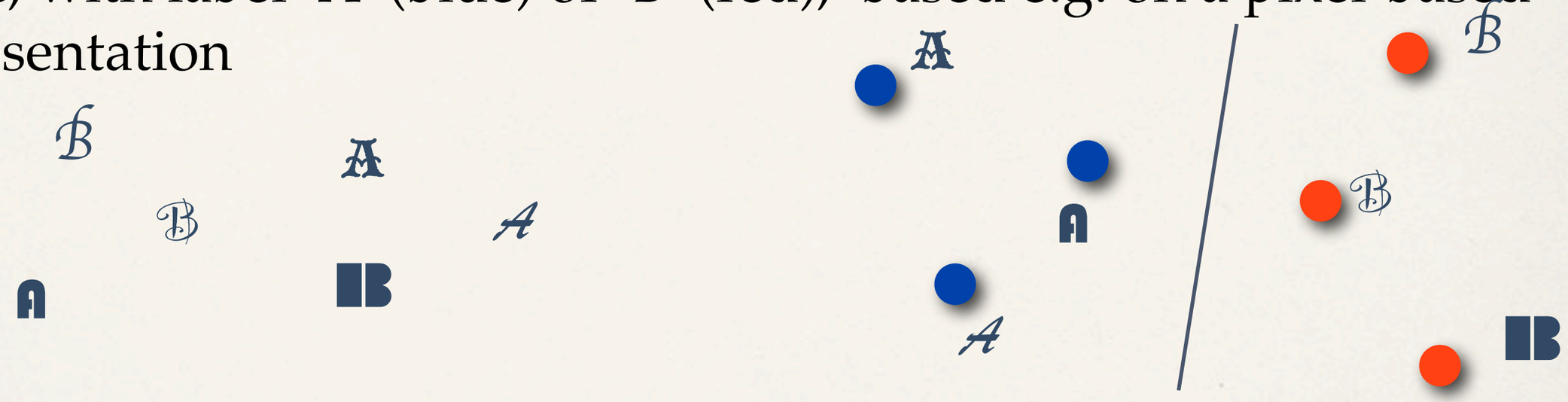

- Separate the 'A's from the 'B's by a simple shape, for example the *maximum-margin hyperplane* (separating hyperplane of maximum distance to any point).

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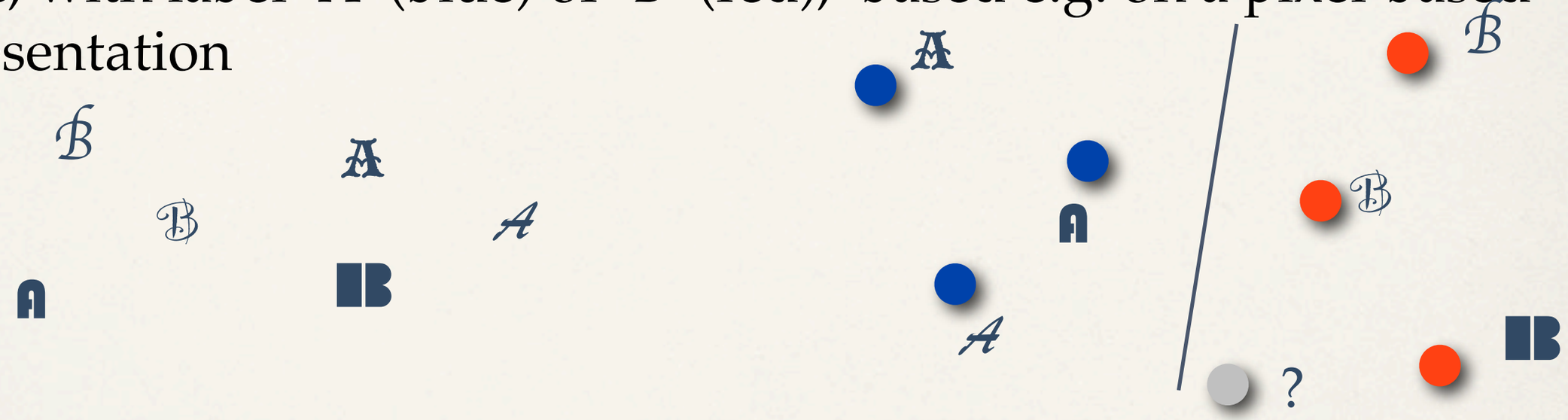


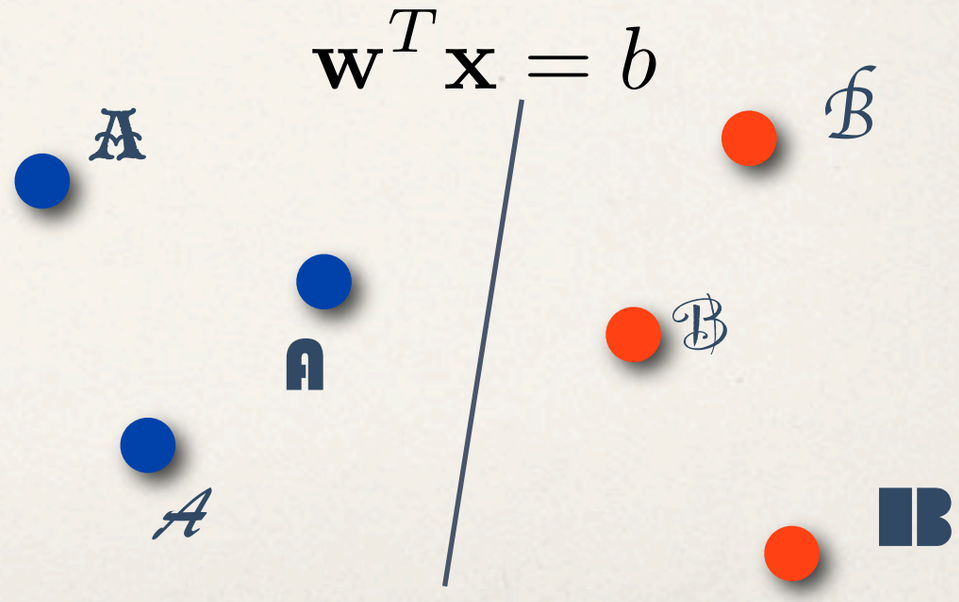
- Separate the 'A's from the 'B's by a simple shape, for example the *maximum-margin hyperplane* (separating hyperplane of maximum distance to any point).

- Classify an unknown letter according to this hyperplane (= 'B')

Support Vector Machines
The primal program

- Computation of Maximum-Margin Hyperplane is a **convex quadratic program:**

$$\begin{array}{lrcl} \min_{\mathbf{w},b} & \frac{1}{2}\mathbf{w}^T\mathbf{w} & & \\ \text{subject to} & \mathbf{w}^T\mathbf{p}_i - b & \geq & 1, \quad \mathbf{p}_i \in A \\ & \mathbf{w}^T\mathbf{p}_i - b & \leq & 1, \quad \mathbf{p}_i \in B \end{array}$$



$$\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n$$

Support Vector Machines
The primal program, class labels

- Computation of Maximum-Margin Hyperplane is a **convex quadratic program:**

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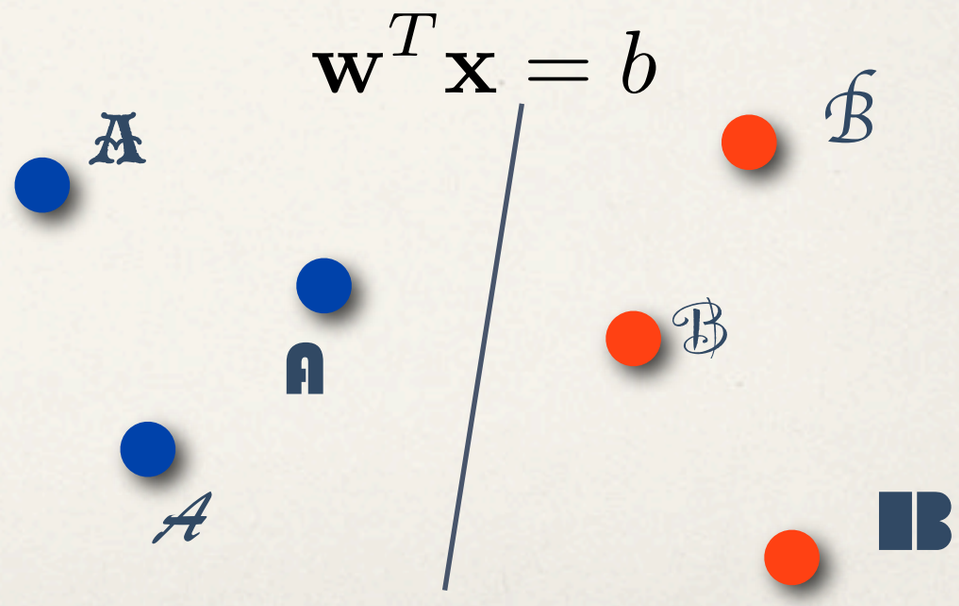
$$y_i = \begin{cases} +1, & \mathbf{p}_i \in A \\ -1, & \mathbf{p}_i \in B \end{cases}$$



$$\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n$$

Support Vector Machines
Dual program

$$
\begin{array}{lll}
\min_{\lambda_i} & \|\mathbf{p}-\mathbf{q}\|^2 & \\
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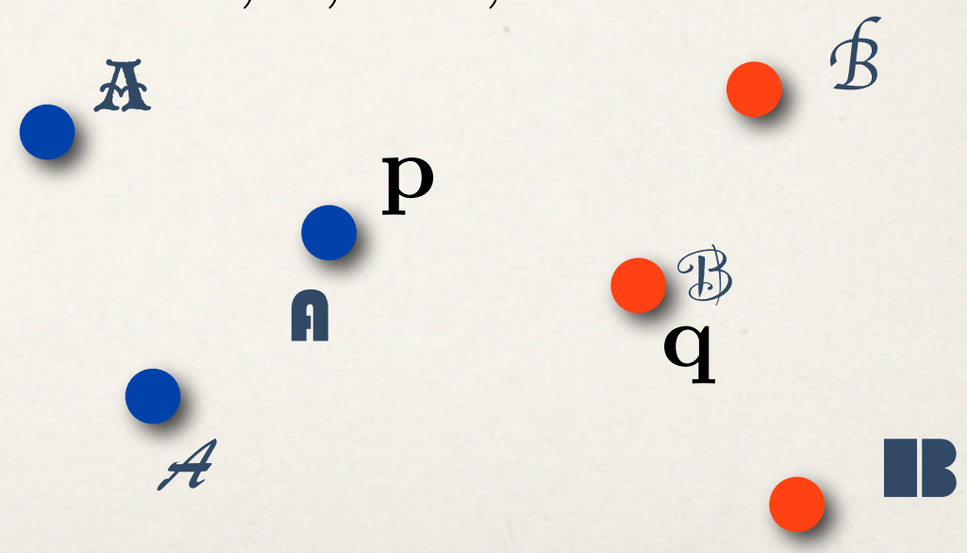

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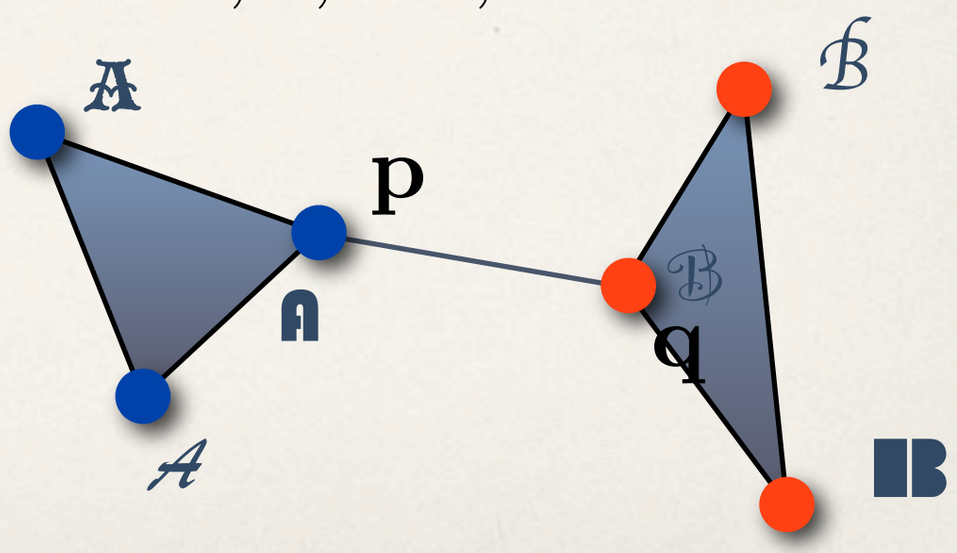
Geometrically, this is the problem of finding the distance between the two polytopes $conv(A)$ and $conv(B)$



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The points with positive λ_i are the *support vectors*

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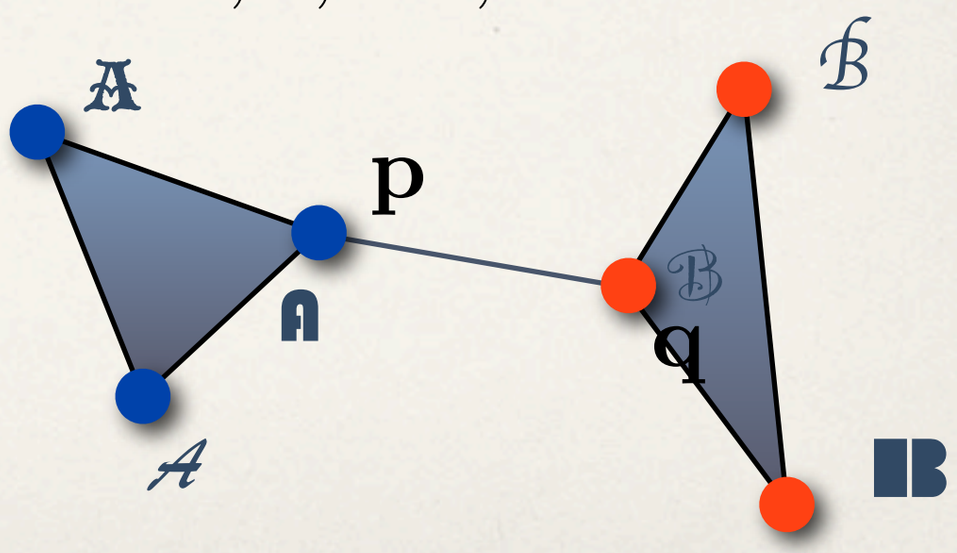

Support Vector Machines
Dual program, class labels

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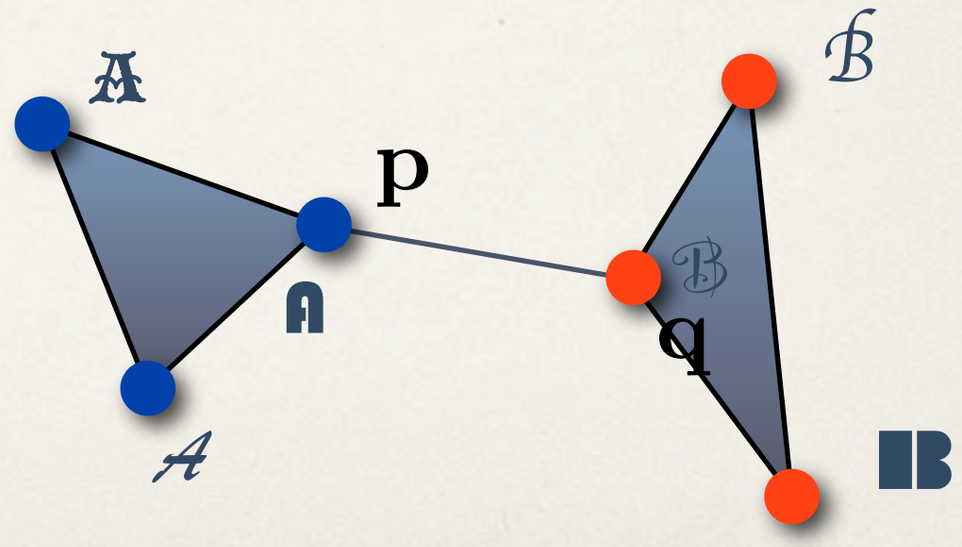

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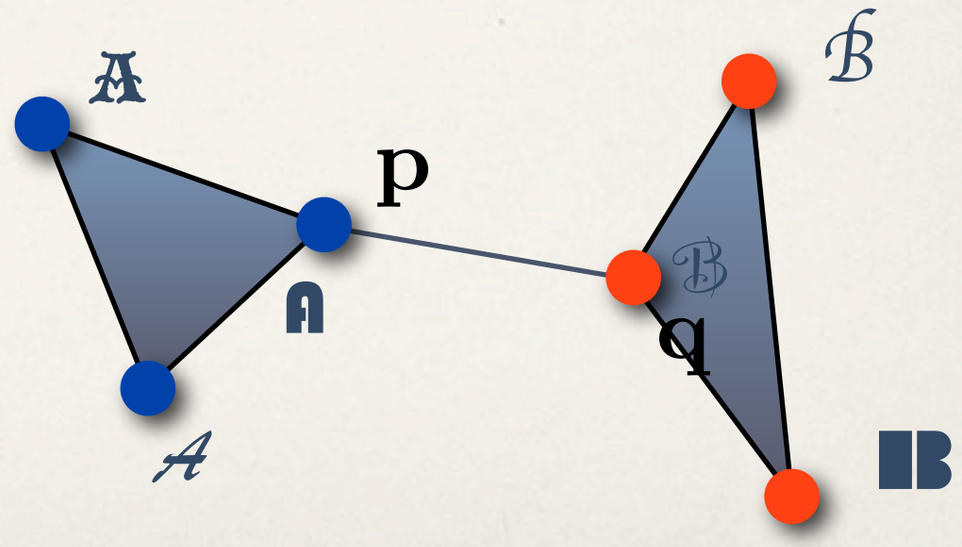
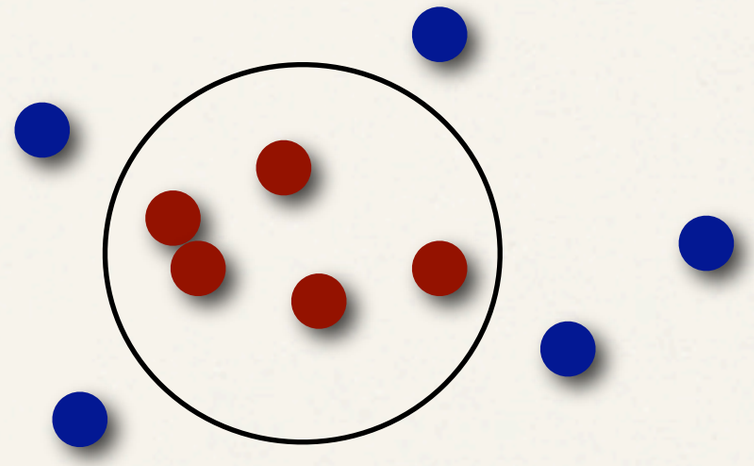
\end{array}
$$

The dual program does not need to know the points, just their pairwise scalar products!



Support Vector Machines
Nonlinear separators

- Other separating shapes (e.g. spheres) may be the "right" shapes for the given problem



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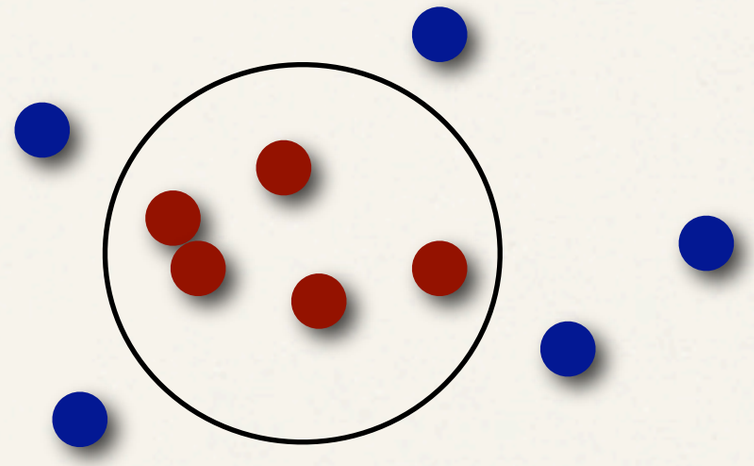


- Apply *lifting* to reduce to separating hyperplane in higher dimension!

Support Vector Machines
Circular Separators

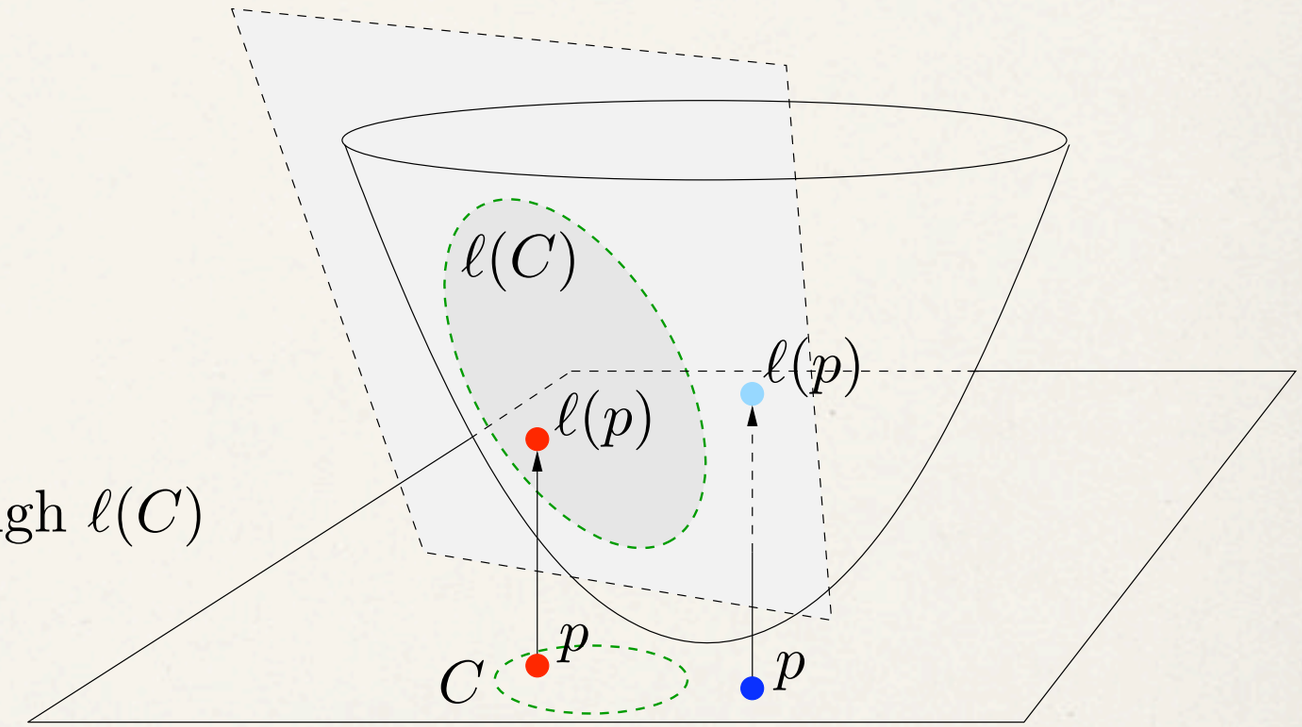
- Apply *lifting map*

$$\ell : (x, y) \mapsto (x, y, x^2 + y^2)$$

$$p \left\{ \begin{array}{l} \text{inside} \\ \text{on} \\ \text{outside} \end{array} \right\} C$$

$$\Updownarrow$$

$$\ell(p) \left\{ \begin{array}{l} \text{below} \\ \text{on} \\ \text{above} \end{array} \right\} \text{the plane through } \ell(C)$$



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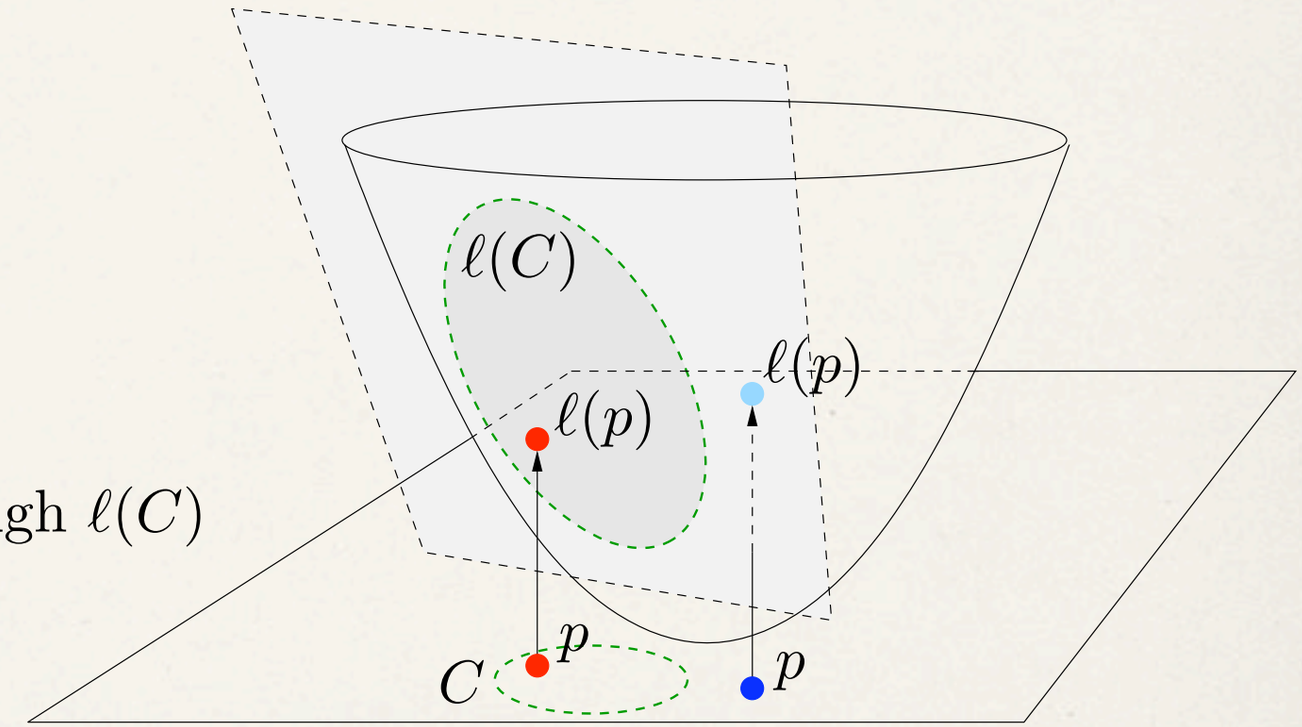

- Use preimage of maximum-margin hyperplane in lifted space

Support Vector Machines
Circular Separators

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- Dual quadratic program becomes

$$\begin{array}{lll} \min_{\lambda_i} & \sum_{i,j} \lambda_i \lambda_j y_i y_j k(\mathbf{p}_i, \mathbf{p}_j) & \\ \text{subject to} & \sum_{\mathbf{p}_i \in A} \lambda_i = 1 & \\ & \sum_{\mathbf{p}_i \in B} \lambda_i = 1 & \\ & \lambda_i \geq 0 & i = 1, 2, \ldots, n \end{array}$$

$$k(\mathbf{p}, \mathbf{q}) = \mathbf{p}_x \mathbf{q}_x + \mathbf{p}_y \mathbf{q}_y + (\mathbf{p}_x^2 + \mathbf{p}_y^2)(\mathbf{q}_x^2 + \mathbf{q}_y)^2$$

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Support Vector Machines
Kernel Trick

- Let $k : \mathbf{R}^d \times \mathbf{R}^d \to \mathbf{R}$ be symmetric and positive semidefinite, meaning that

$$\sum_{i,j} \lambda_i \lambda_j k(\mathbf{p}_i, \mathbf{p}_j) \geq 0, \quad \forall \mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n, \lambda_1, \lambda_2, \ldots, \lambda_n$$

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The quadratic program implicitly computes the maximum-margin hyperplane in H

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- Compute $\mathbf{w}^T \mathbf{x} - b$, where $\mathbf{w}^T \mathbf{x} = \sum_i \lambda_i y_i k(\mathbf{p}_i, \mathbf{x})$

support vector

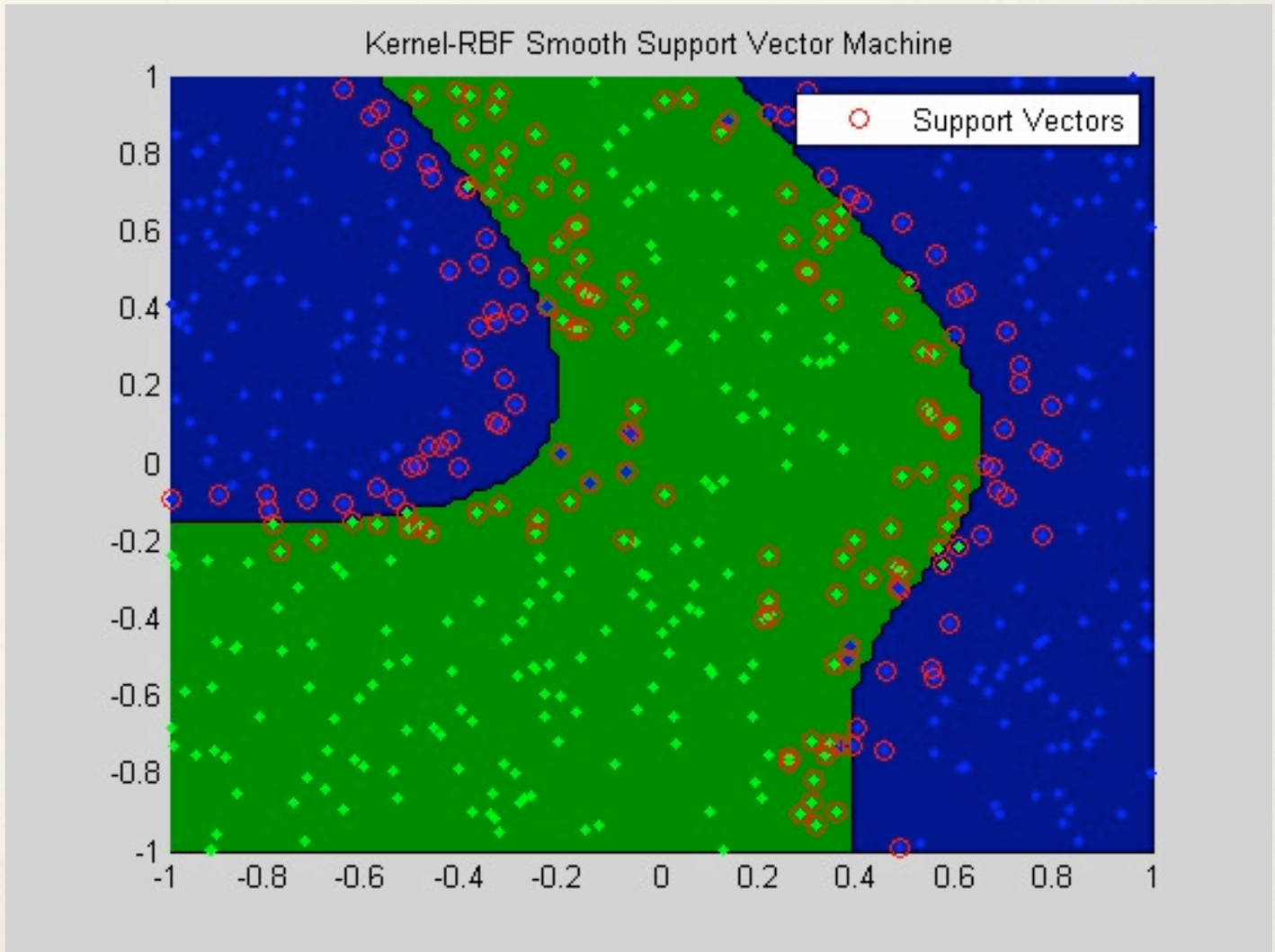
$$b = \sum_i^i \lambda_i y_i k(\mathbf{p}_i, \mathbf{p}_j) - y_j$$

Support Vector Machines
Kernel Trick

- Visualization of nonlinear separator in original space

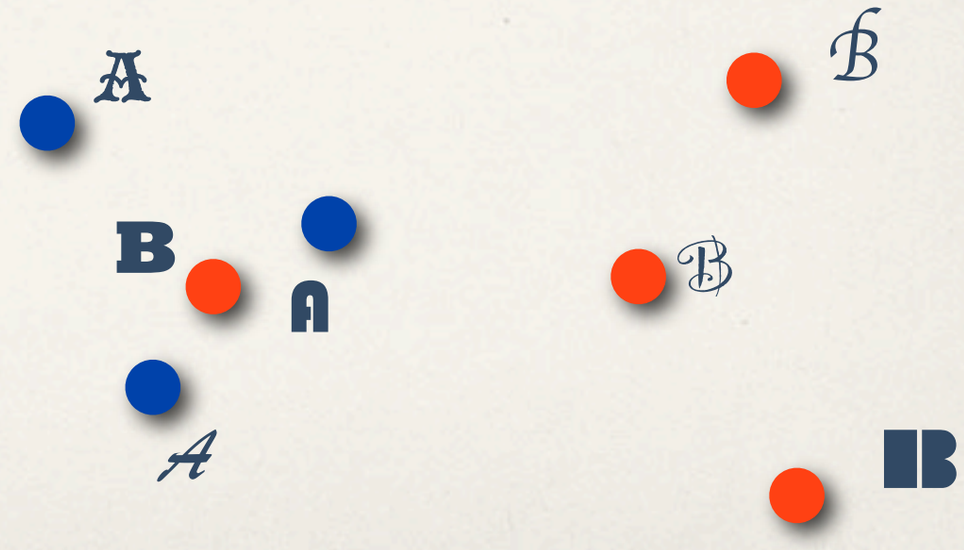
$$k(\mathbf{p}, \mathbf{q}) = e^{-\mu \|\mathbf{p}-\mathbf{q}\|}$$

"Radial Basis Function" (RBF)



Support Vector Machines
Soft Margin

- In many cases, a proper separation cannot be expected, due to noise and outliers



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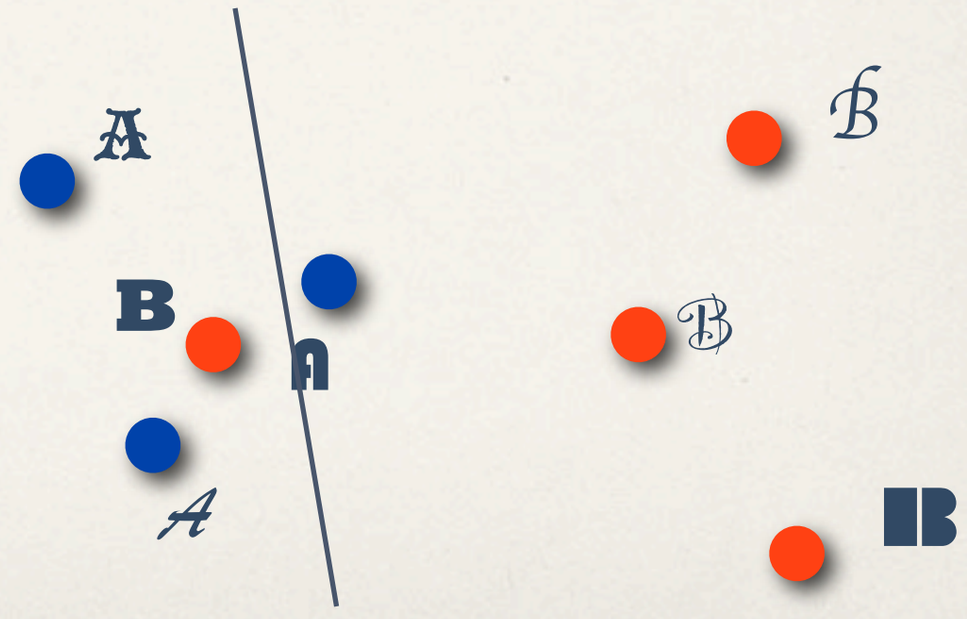
- Allow misclassifications of training points, but penalize them!



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- ν-SVM, where ν is a fixed parameter

$$
\begin{array}{lllll}
\min_{\mathbf{w},b,\rho,\xi_i} & \frac{1}{2}\mathbf{w}^T\mathbf{w} - \nu\rho & + & \frac{1}{n}\sum_{i=1}^{n}\xi_i & \\
\text{subject to} & y_i(\mathbf{w}^T\mathbf{p}_i - b) & \geq & \rho - \xi_i, & i = 1, 2, \ldots, n \\
& \xi_i & \geq & 0, & i = 1, 2, \ldots, n \\
& \rho & \geq & 0 &
\end{array}
$$

previously,
we had 1 here

Support Vector Machines
Soft Margin

- In many cases, a proper separation cannot be expected, due to noise and outliers

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- dual ν-SVM (with $\mu := \frac{2}{n\nu}$):

$$
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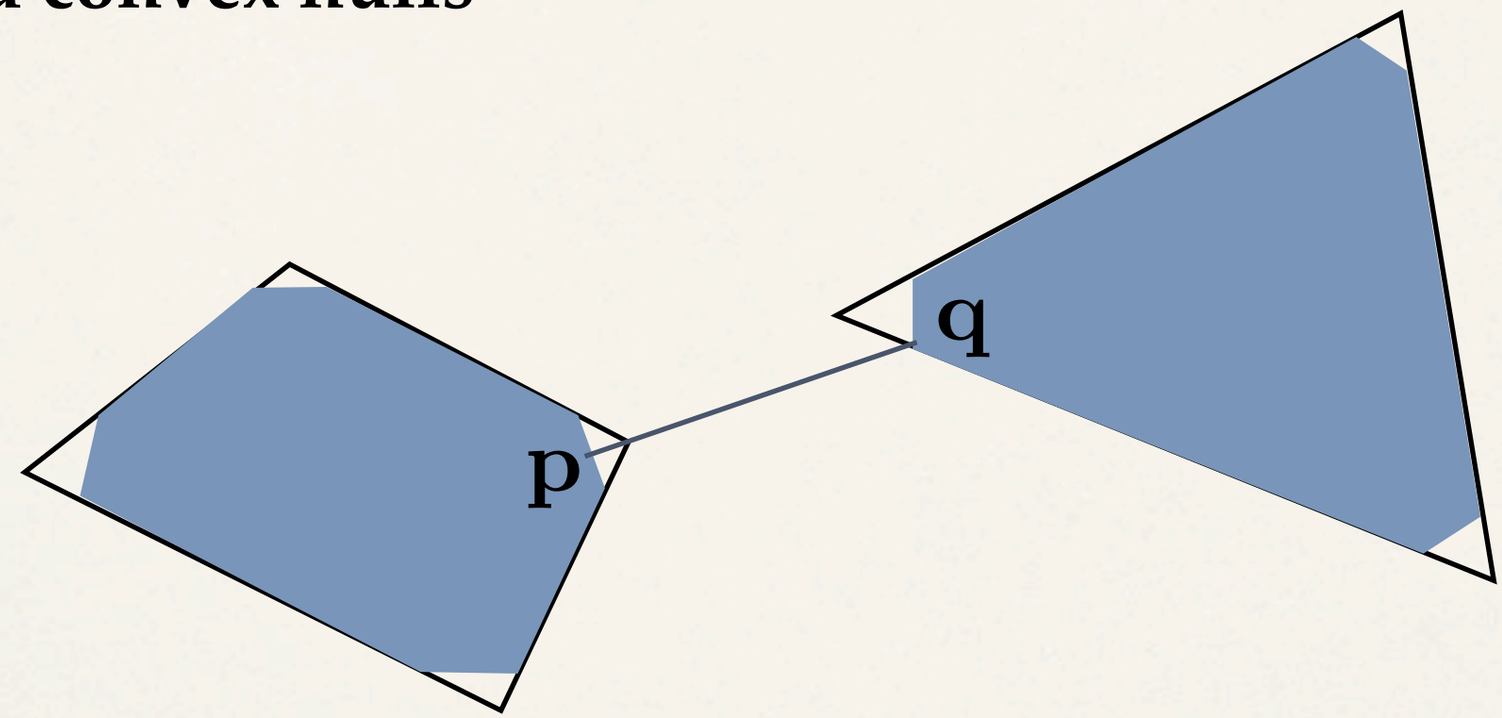
& \sum_{\mathbf{p}_i \in B} \lambda_i = 1 & \\
& \lambda_i \geq 0 & i = 1, 2, \ldots, n \\
\text{new} \longrightarrow & \lambda_i \leq \mu & i = 1, 2, \ldots, n
\end{array}
$$

Support Vector Machines
Soft Margin: The Geometric View

- The dual ν-SVM is the problem of finding the distance between two **reduced convex hulls**



Support Vector Machines
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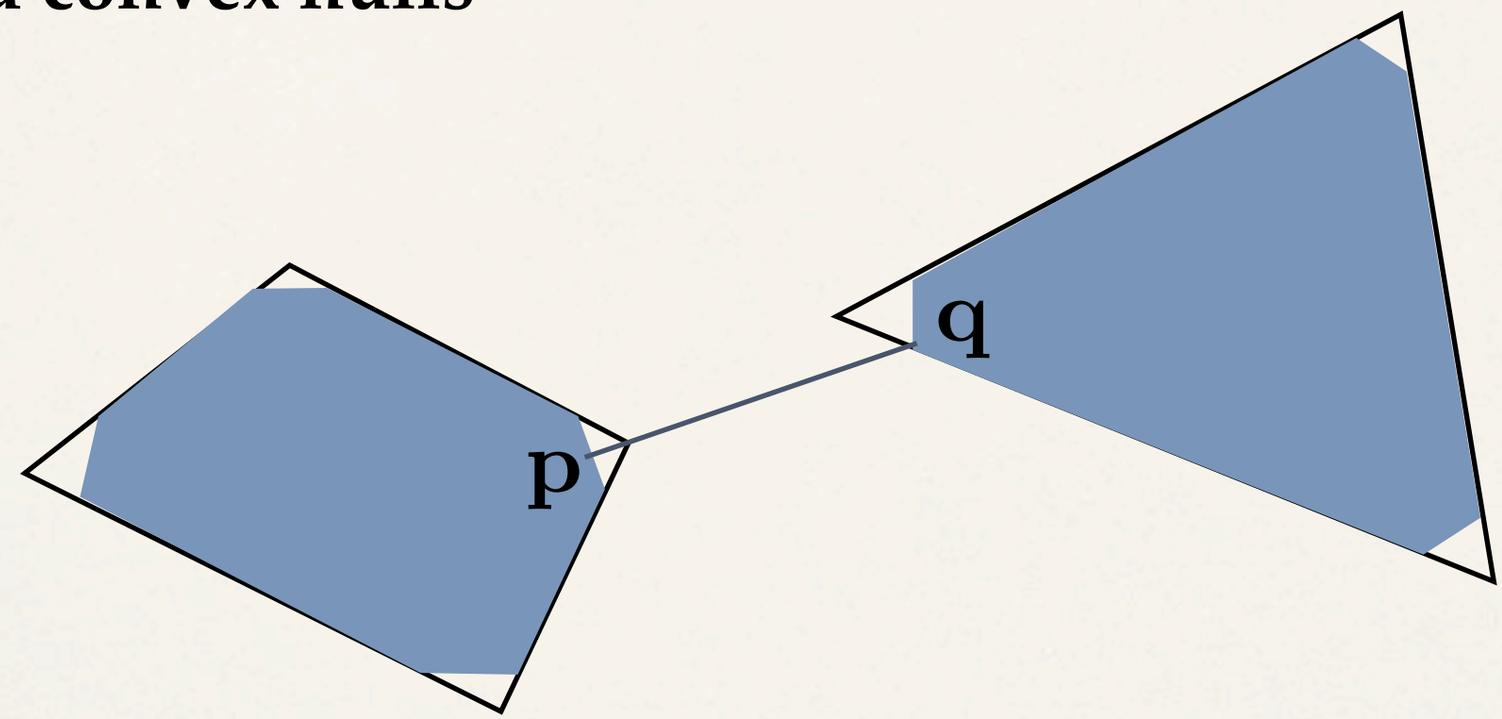
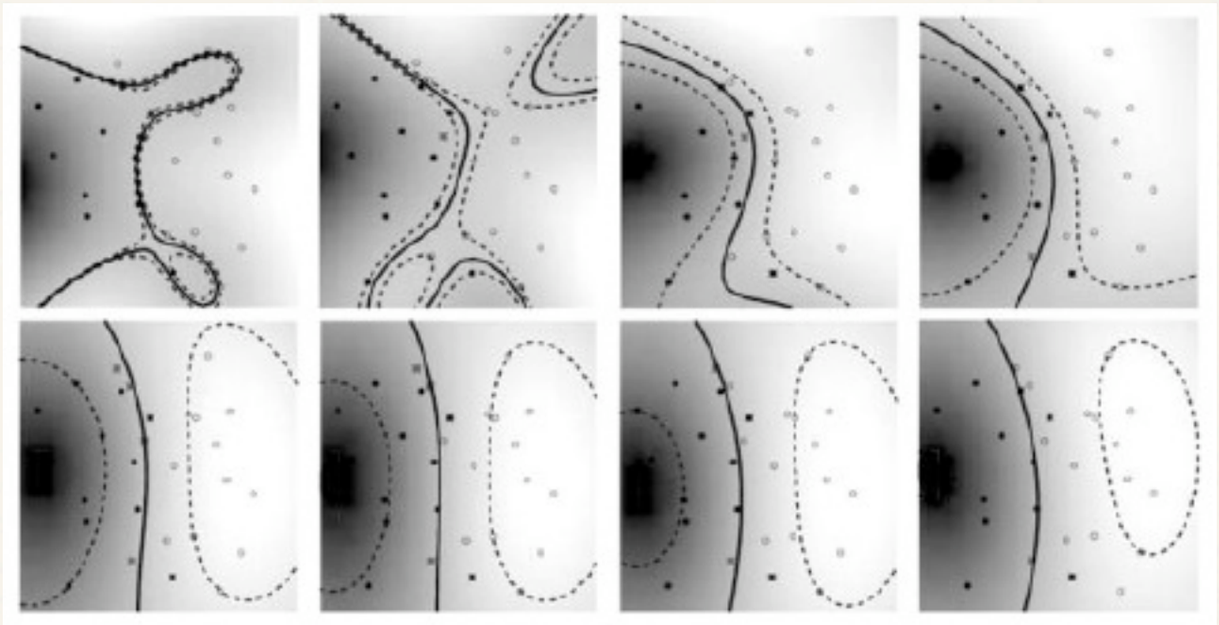


- $\mu = 1$: no reduction

$\mu = 1/2$: edges start to disappear

Support Vector Machines
Soft Margin: Parameter Choice

- How does ν (or μ in the dual) influence the separator?



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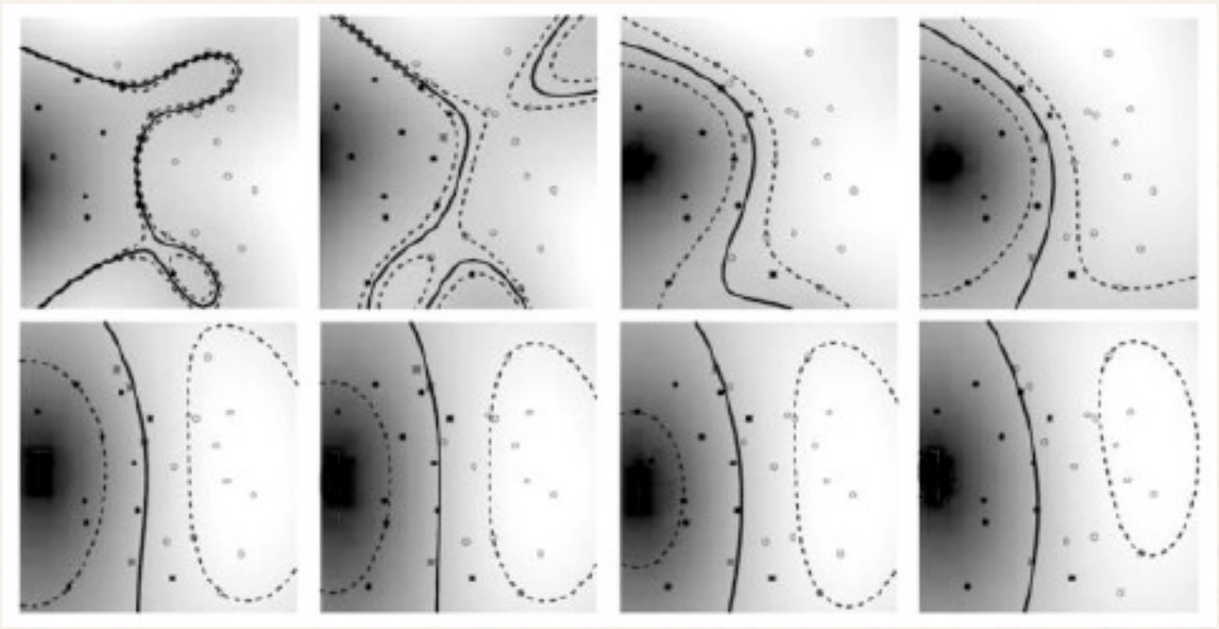
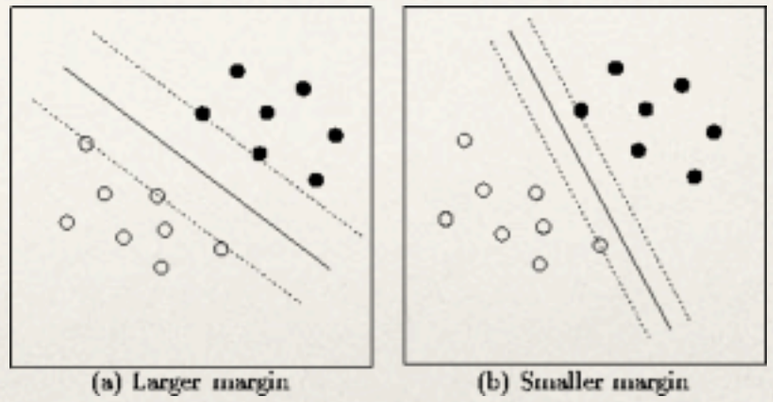


- Small ν: small margin (**overfitting)**
- Large ν: large margin (**underfitting**)



Support Vector Machines
Soft Margin: Parameter Choice

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- Standard method: **grid search** (discretize the relevant parameter range and try all values in the discretized range; one QP per value)

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Soft Margin: Parameter Choice

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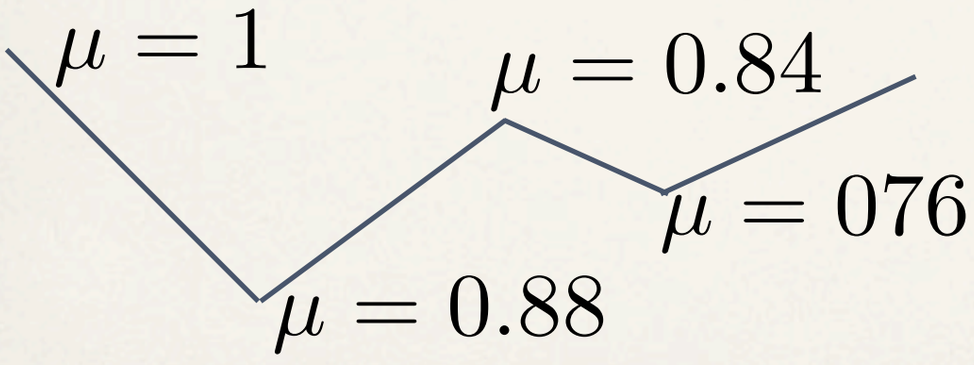
- Standard method: **grid search** (discretize the relevant parameter range and try all values in the discretized range; one QP per value)

- Solution path method: compute the solution of the dual SVM as a piecewise linear function in μ, then grid search (one lookup per value)



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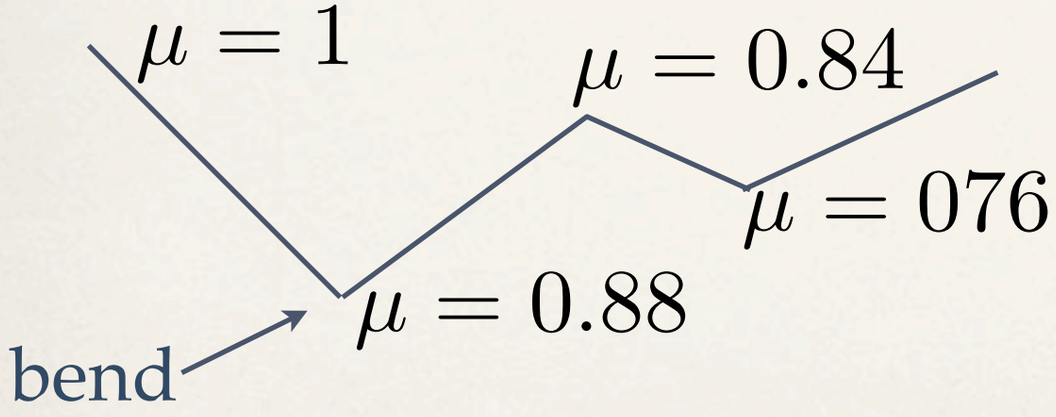
& \lambda_i & \geq & 0 & i = 1, 2, \ldots, n \\
& \lambda_i & \leq & \mu & i = 1, 2, \ldots, n
\end{array}
$$

Support Vector Machines
Soft Margin: Parameter Choice

- How to choose the parameter in a given application?

- Standard method: **grid search** (discretize the relevant parameter range and try all values in the discretized range; one QP per value)

- Solution path method: compute the solution of the dual SVM as a piecewise linear function in μ, then grid search (one lookup per value)



$$
\begin{array}{lllll}
\min_{\lambda_i} & \sum_{i,j} \lambda_i \lambda_j y_i y_j \mathbf{p}_i^T \mathbf{p}_j & & & \\
\text{subject to} & \sum_{\mathbf{p}_i \in A} \lambda_i & = & 1 & \\
& \sum_{\mathbf{p}_i \in B} \lambda_i & = & 1 & \\
& \lambda_i & \geq & 0 & i = 1, 2, \ldots, n \\
& \lambda_i & \leq & \mu & i = 1, 2, \ldots, n
\end{array}
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- Performance depends on the **number of bends** in the solution path

Support Vector Machines
The Hastie et al. Conjecture

- Hastie et al. 2004: *The entire regularization path for the support vector machine*

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- Conjecture was repeatedly stated in other articles, and it was experimentally "confirmed" in a large number of applications

Support Vector Machines The Conjecture is False

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- **Theorem (G., Jaggi, Maria 2010) :** There are point sets A and B in d-dimensional space with $|A| = 2d$, $|B| = 2$, for which the solution path of the dual ν-SVM has an *exponential* number of at least $2^d / 4$ many bends.

Parametric Linear Programs

- **Recall**: primal ν-SVM is a parametric quadratic program (parameter in the objective function):

$$
\begin{array}{lllll}
\min_{\mathbf{w},b,\rho,\xi_i} & \frac{1}{2}\mathbf{w}^T\mathbf{w} - \nu\rho & + & \frac{1}{n}\sum_{i=1}^{n}\xi_i & \\
\text{subject to} & y_i(\mathbf{w}^T\mathbf{p}_i - b) & \geq & \rho - \xi_i, & i = 1, 2, \ldots, n \\
& \xi_i & \geq & 0, & i = 1, 2, \ldots, n \\
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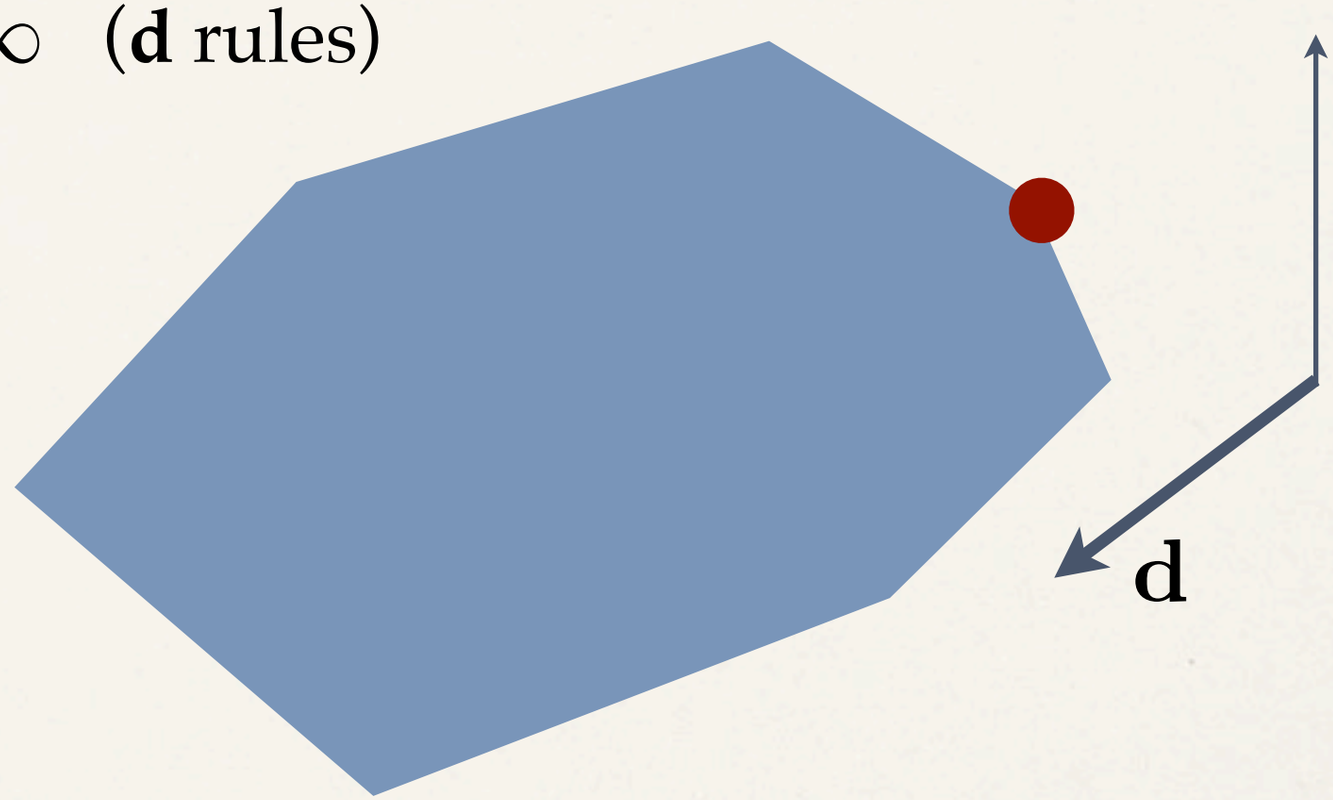
- **Parametric linear program:**

$$\begin{array}{lll} \min & (\mathbf{c}^T + \nu\mathbf{d})^T\mathbf{x} & \\ \text{subject to} & A\mathbf{x} = b & 0 \leq \nu \leq \infty \\ & \mathbf{x} \geq 0 & \end{array}$$

Parametric Linear Programs
The Solution Path

$$\min\ (\mathbf{c}^T + \nu\mathbf{d})^T\mathbf{x}$$

- Start with $\nu = \infty$ (**d** rules)



● = opt

Parametric Linear Programs
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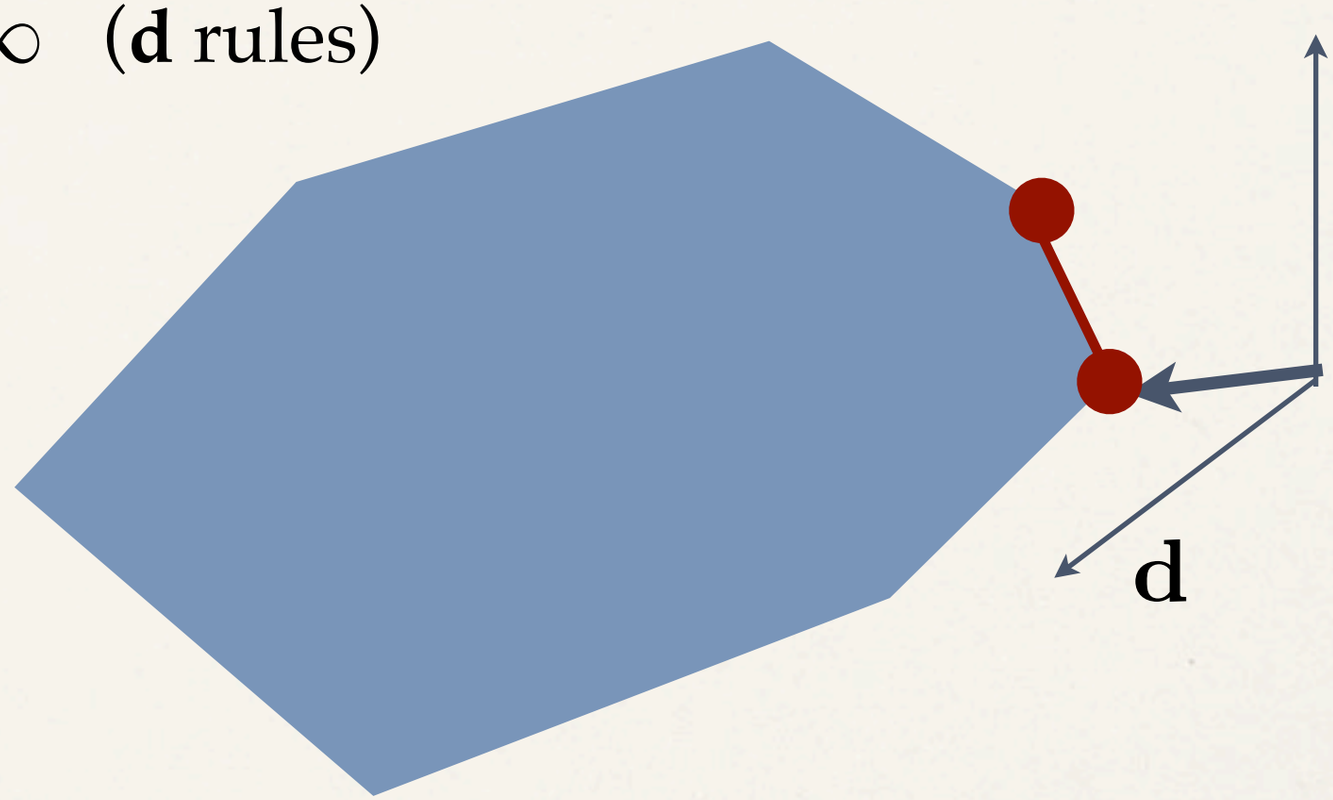

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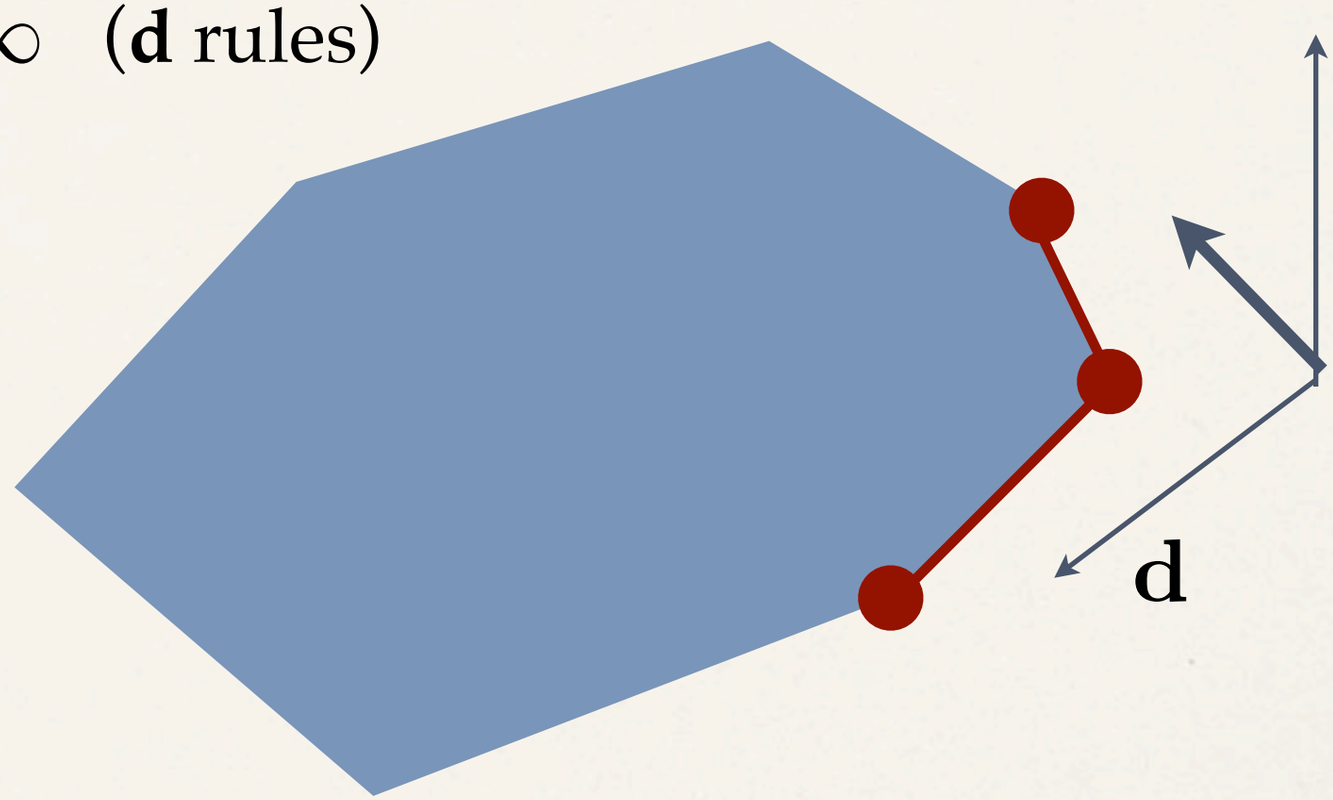

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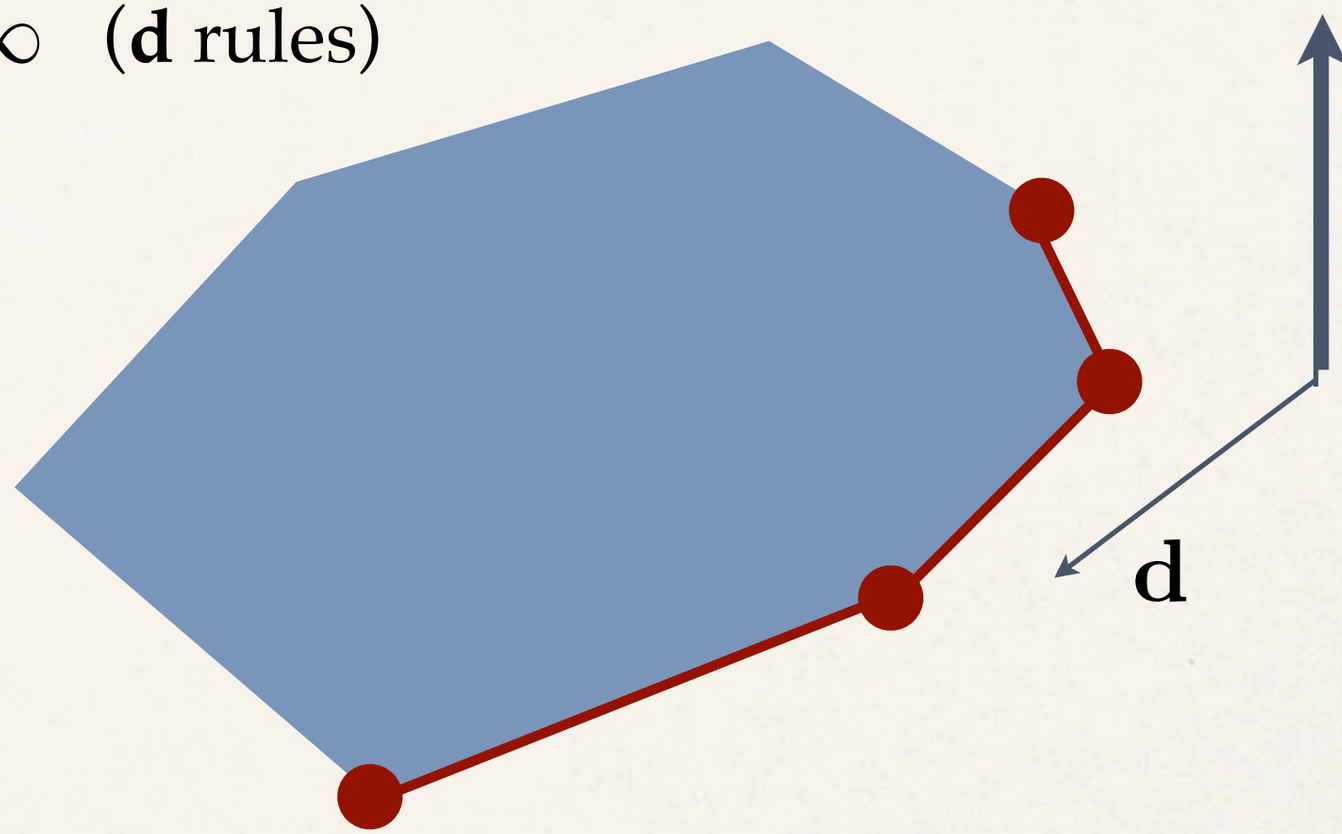

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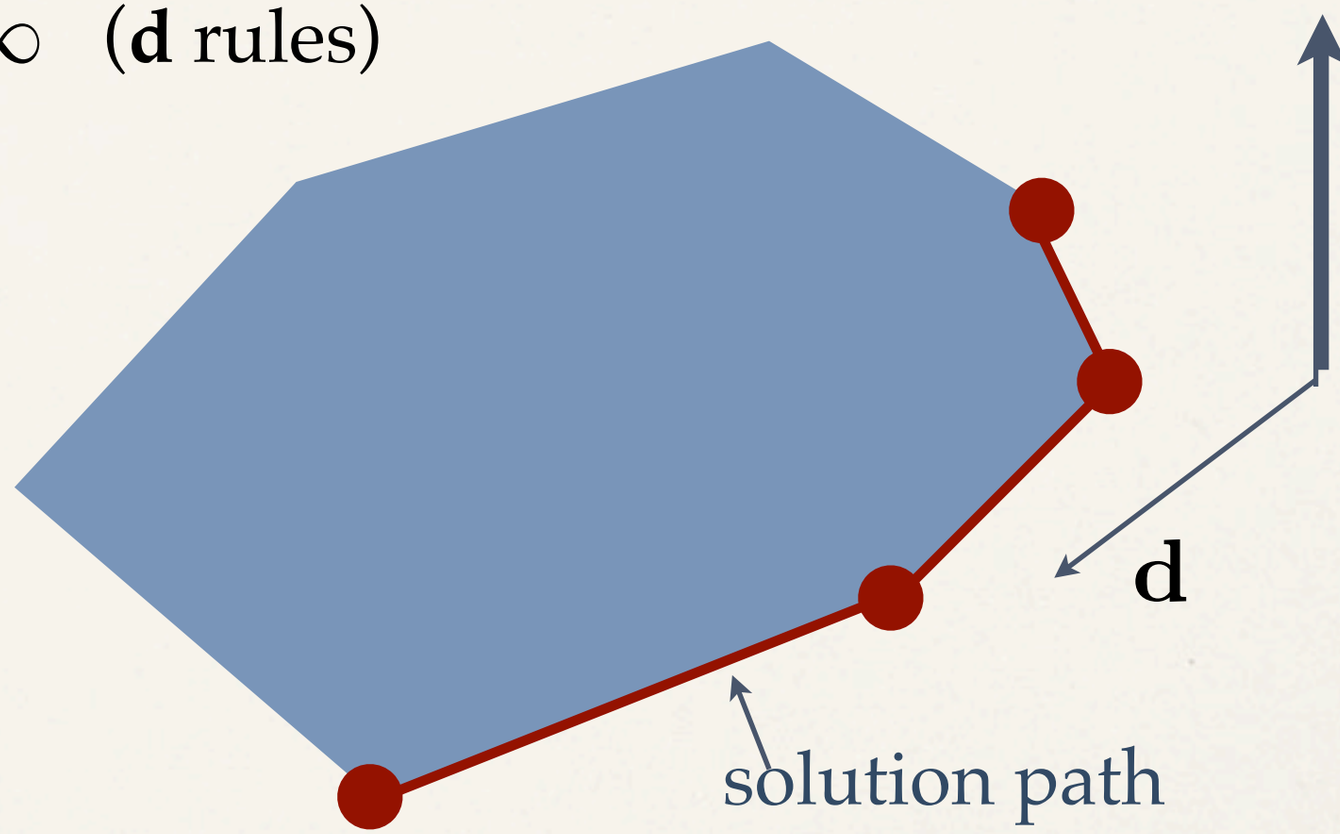

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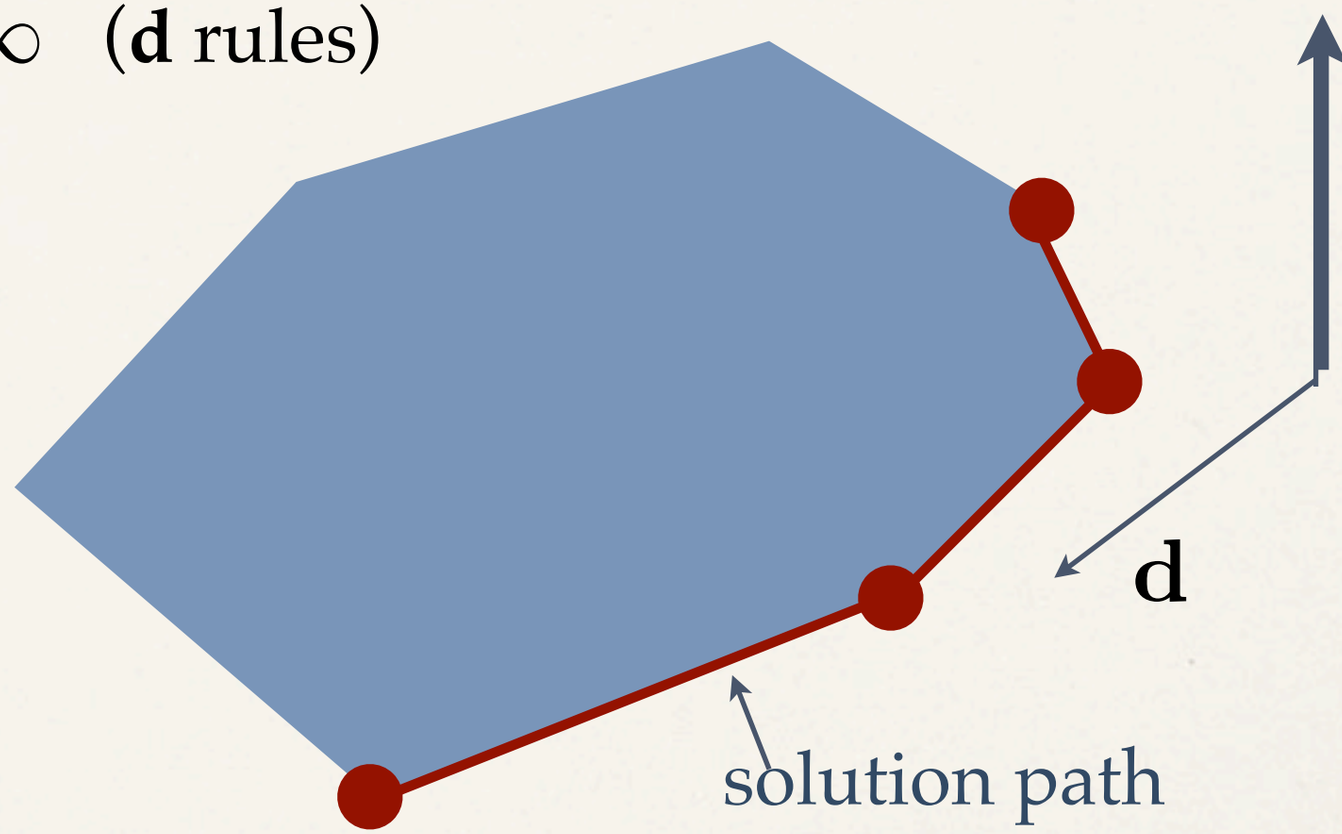
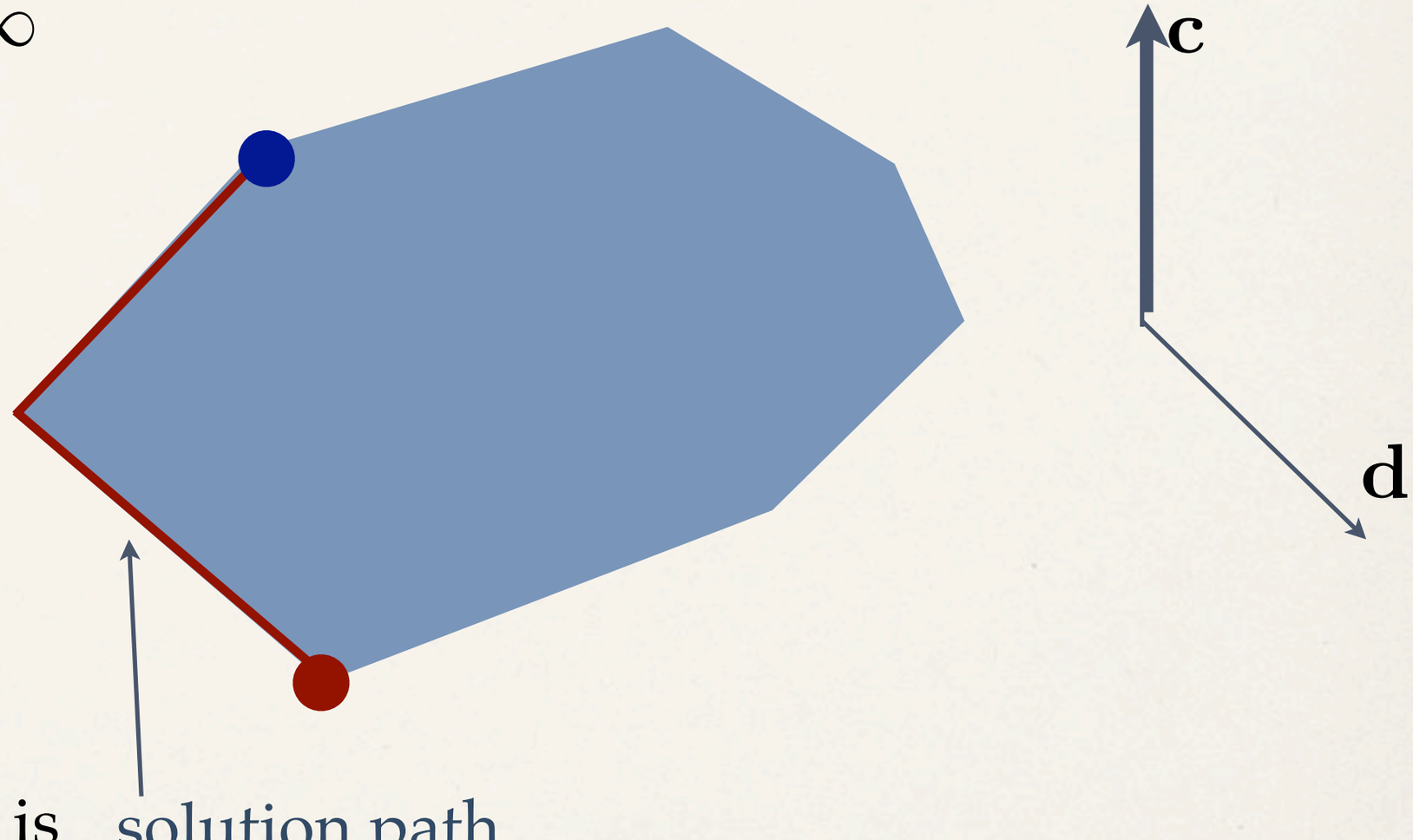


● = opt

- Same picture in higher *d*, with blue polygon the *shadow* of the LP

The Shadow Vertex / Parametric Objective Simplex Algorithm $\min \mathbf{c}^T\mathbf{x}$

- Start with $\nu = \infty$ (and artificial $\mathbf{d}$ such that start vertex ● is optimal)
- Decrease ν...
- until $\nu = 0$
- Vertex ● obtained is optimal under $\mathbf{c}$



The Goldfarb Cubes

- Worst case inputs for the shadow vertex simplex algorithm
- The d-dimensional Goldfarb cube is a deformed unit cube with all its 2^d vertices appearing on a 2-dimensional shadow

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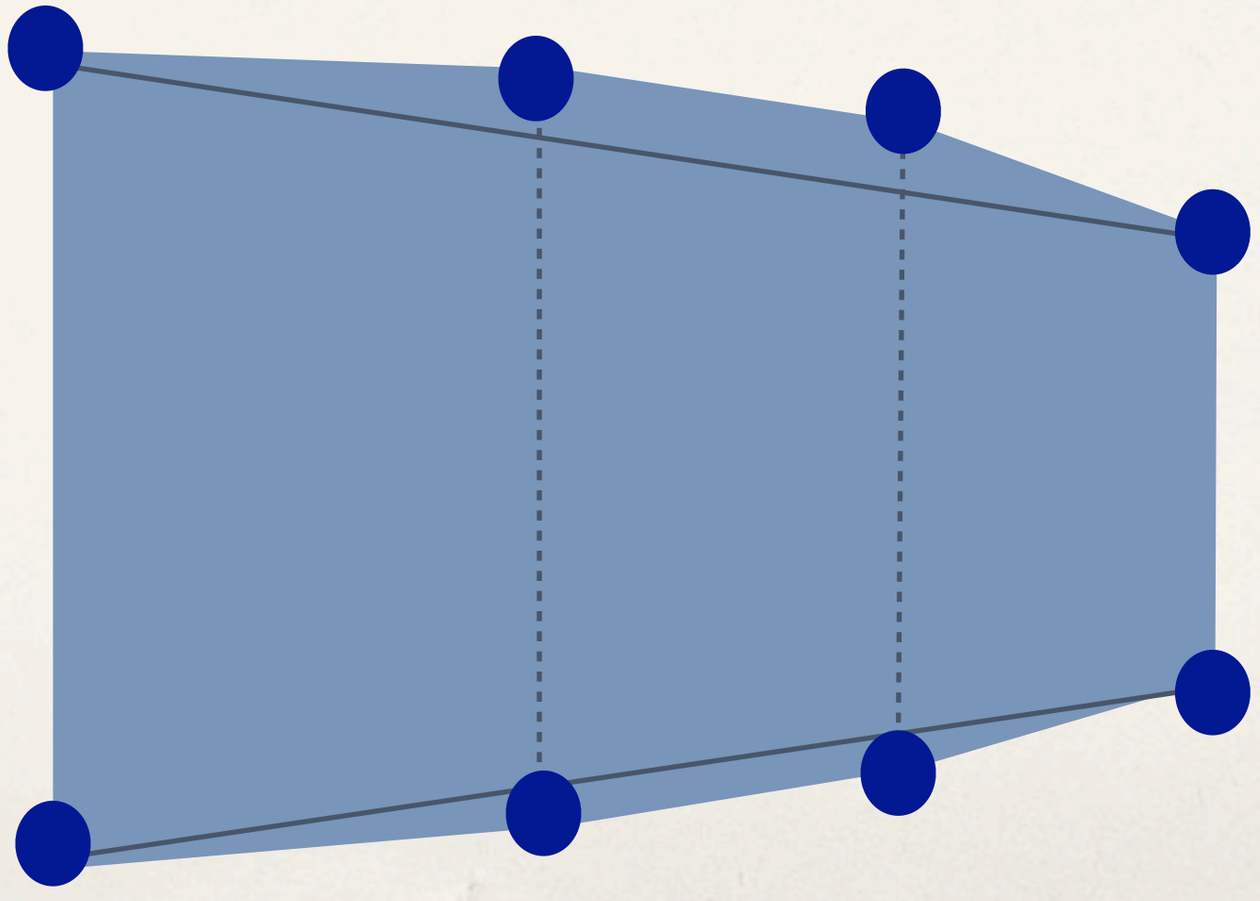
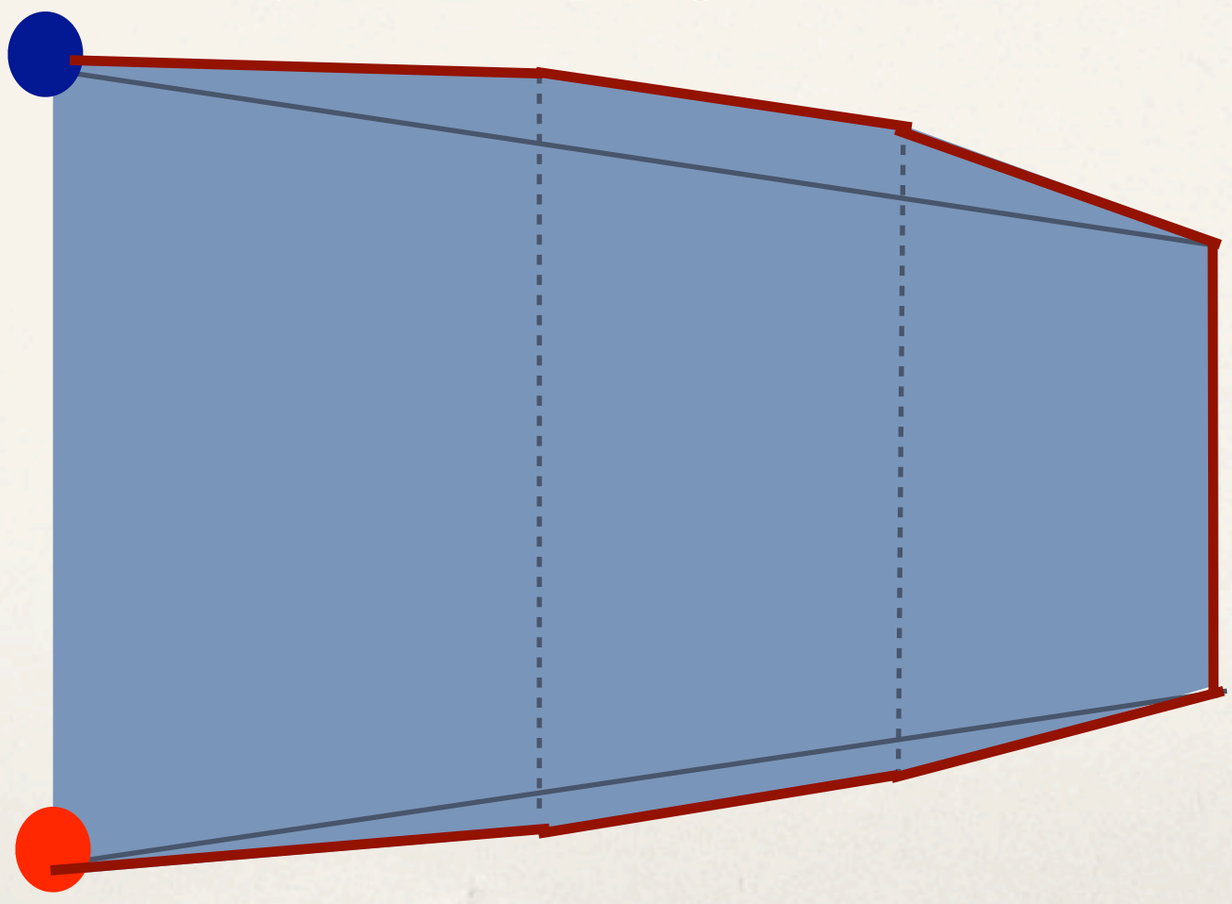


Solution Paths of Parametric Linear Programs...

- can be exponentially long in the worst case
- It is not implausible that a similar result holds for the solution path of SVM (specific parametric *quadratic* programs)



Solution Paths of Parametric Linear Programs...

- can be exponentially long in the worst case
- It is not implausible that a similar result holds for the solution path of SVM (specific parametric *quadratic* programs)
- **Obstacles:**
  - SVM are very special parametric quadratic programs
  - Goldfarb cube is not an instance of an SVM
  - we want a *nondegenerate* SVM with a long solution path

An SVM with an Exponentially Long Solution Path

- **Outline:**
  - Work in the dual (μ-SVM: distance between reduced convex hulls)

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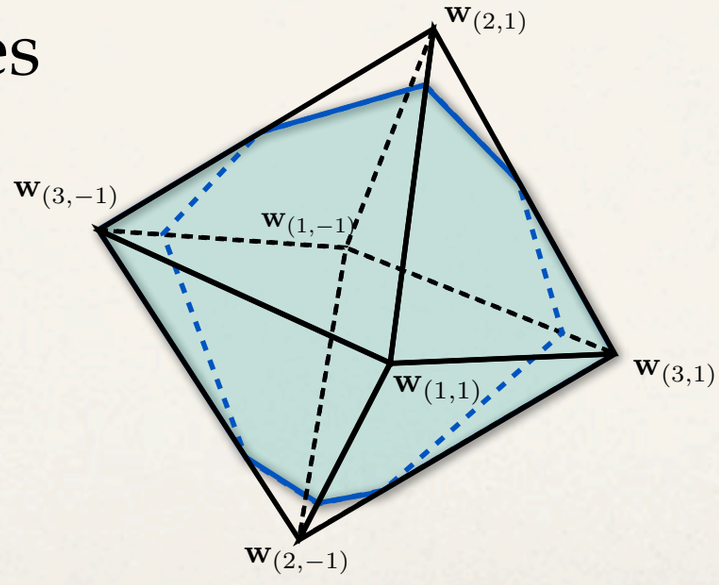

3d

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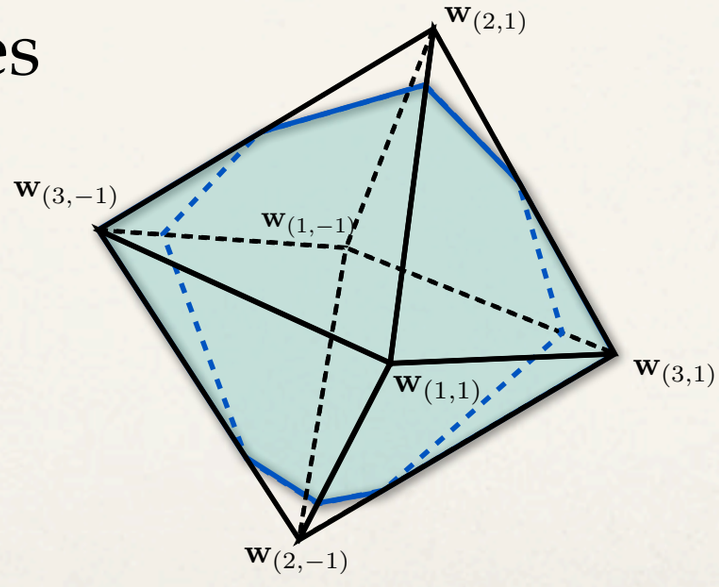
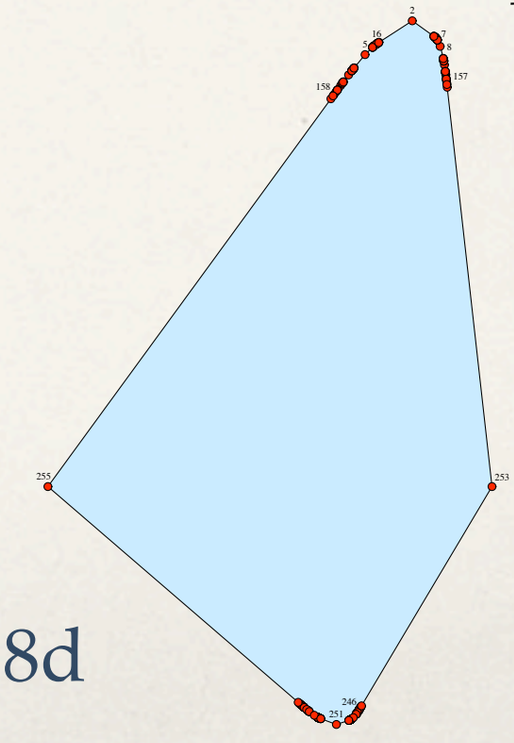


3d



8d

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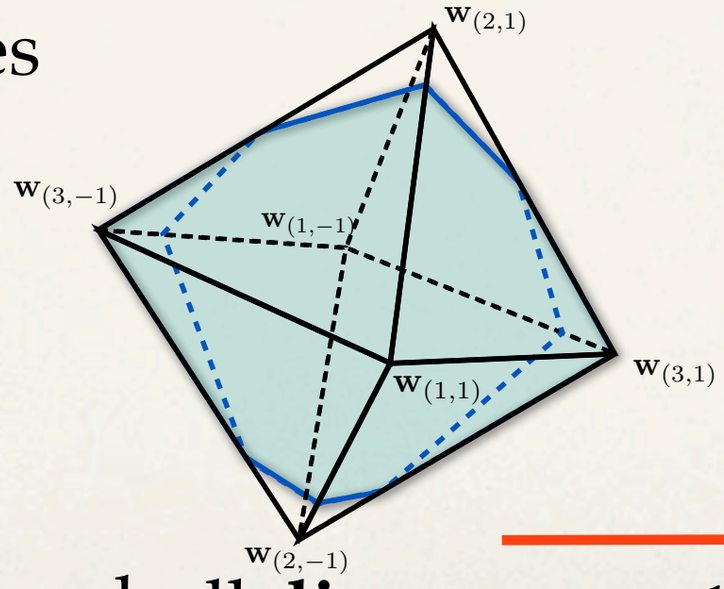

  - Second convex hull: **line segment in S**

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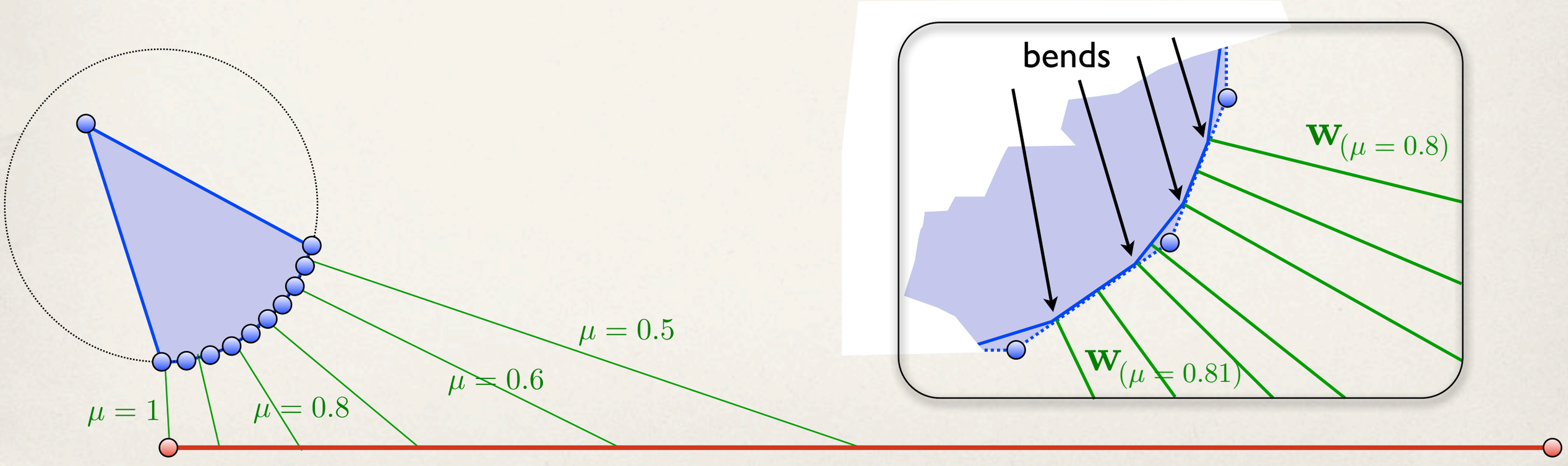
- **Outline:**
  - While μ decreases, the left segment endpoint moves to the right (reduction!). The shortest distance vector traverses 2^d / 4 many edges of the dual Goldfarb cube intersection with S



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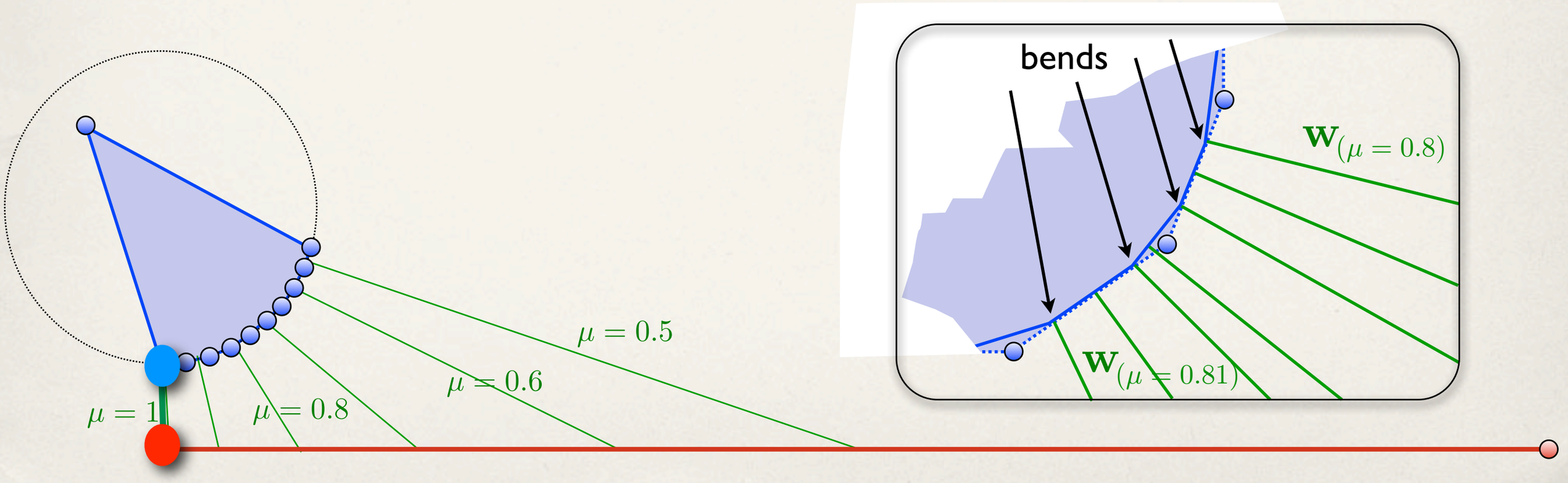

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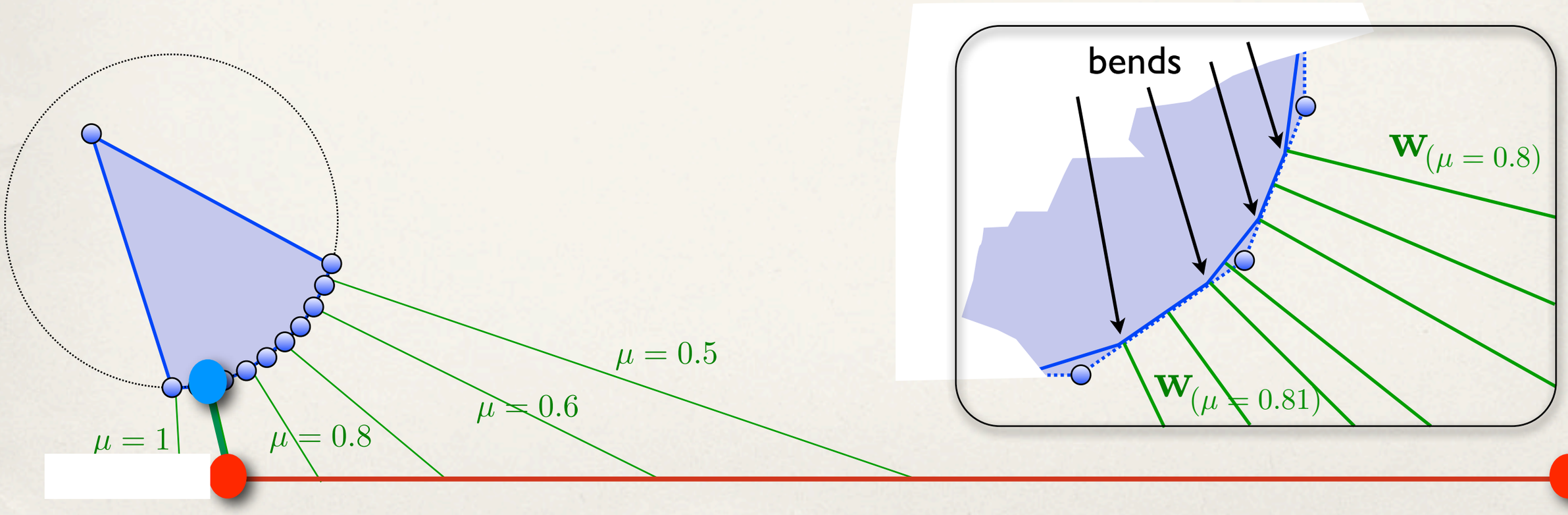

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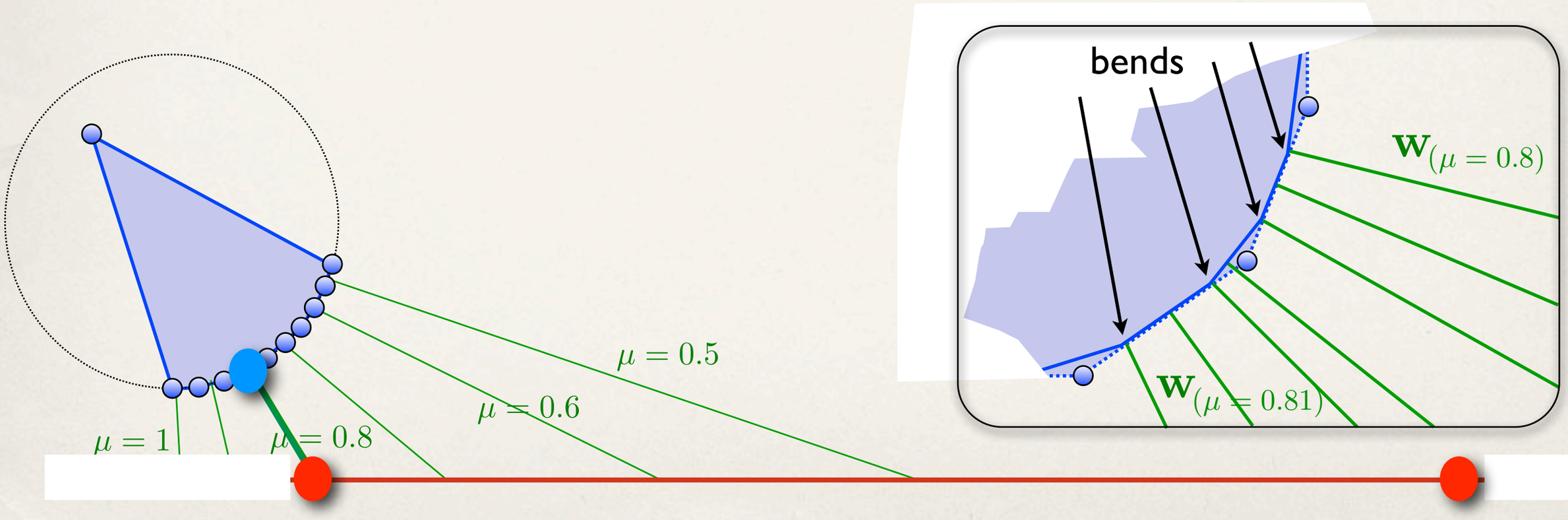

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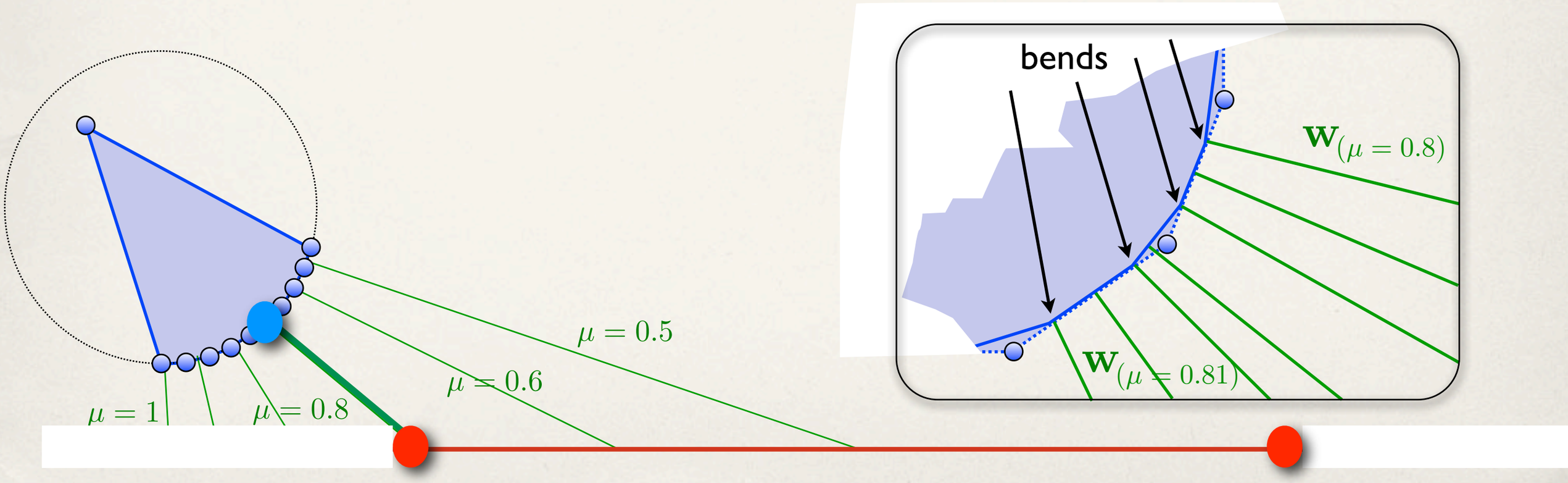

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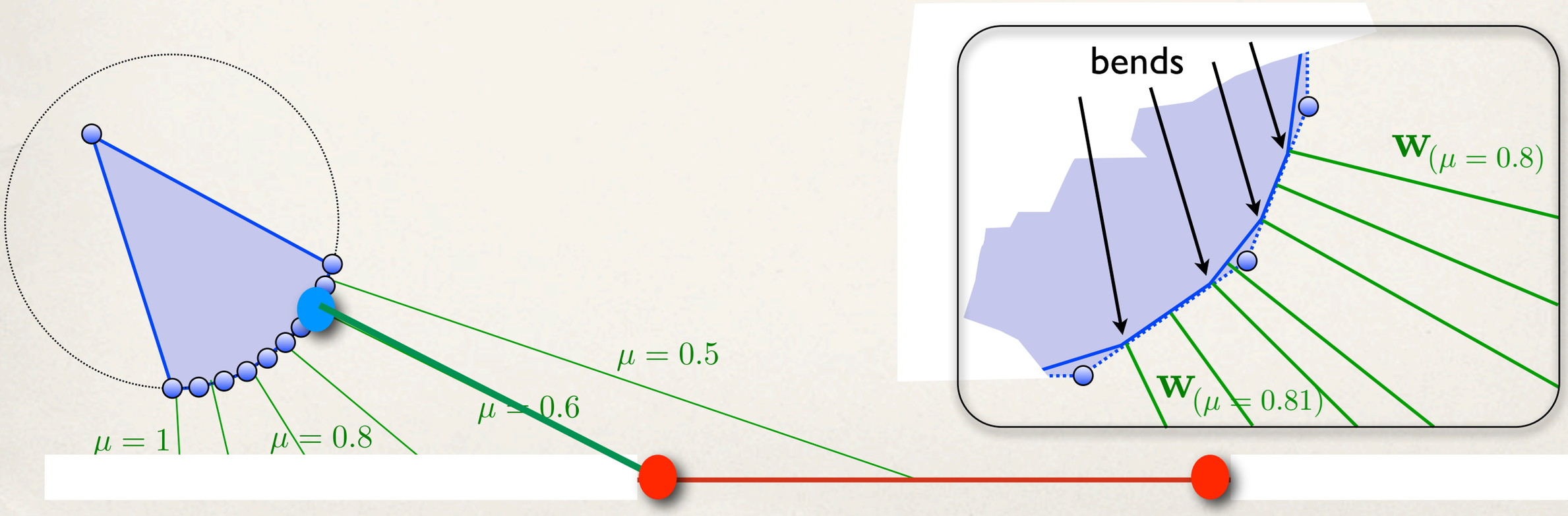

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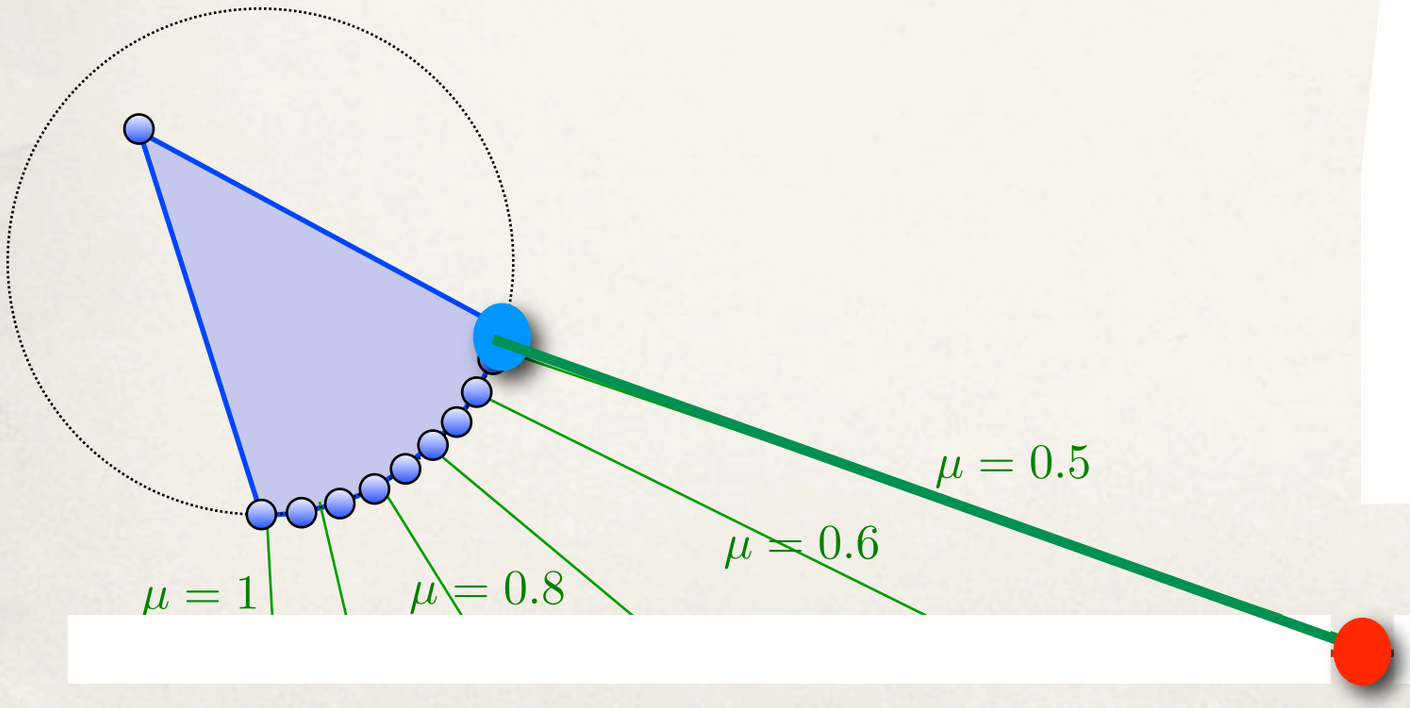
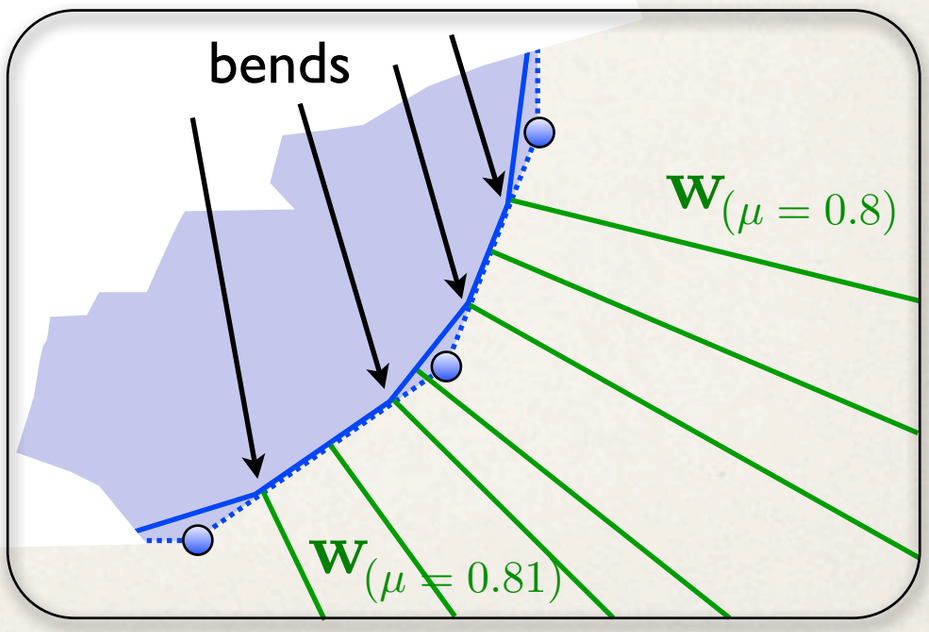
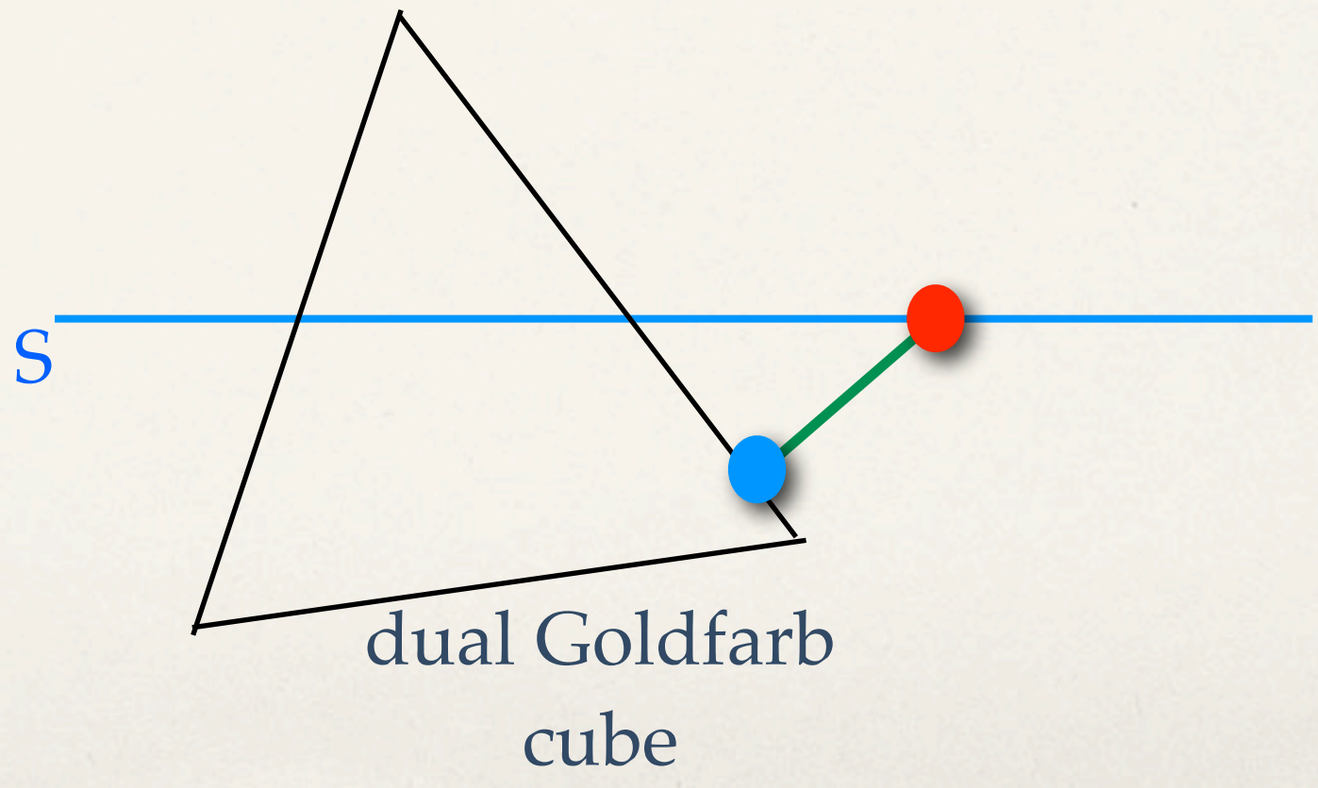




An SVM with an Exponentially Long Solution Path

- **Technical difficulties:**
  - Point of optimal distance in the dual Goldfarb cube may be far away from S and does not "walk along" S



An SVM with an Exponentially Long Solution Path

- **Technical difficulties:**
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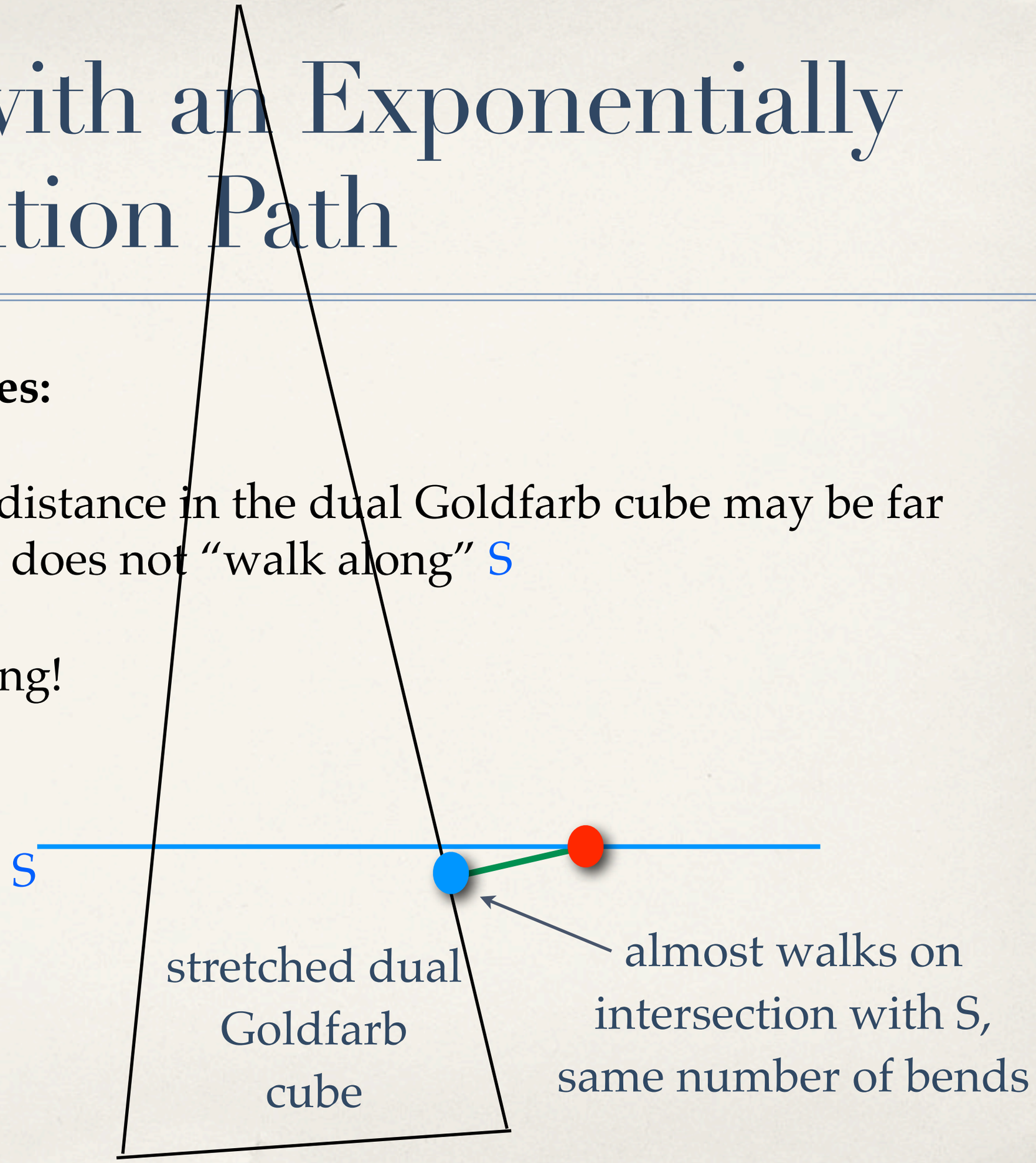
- Solution: stretching!



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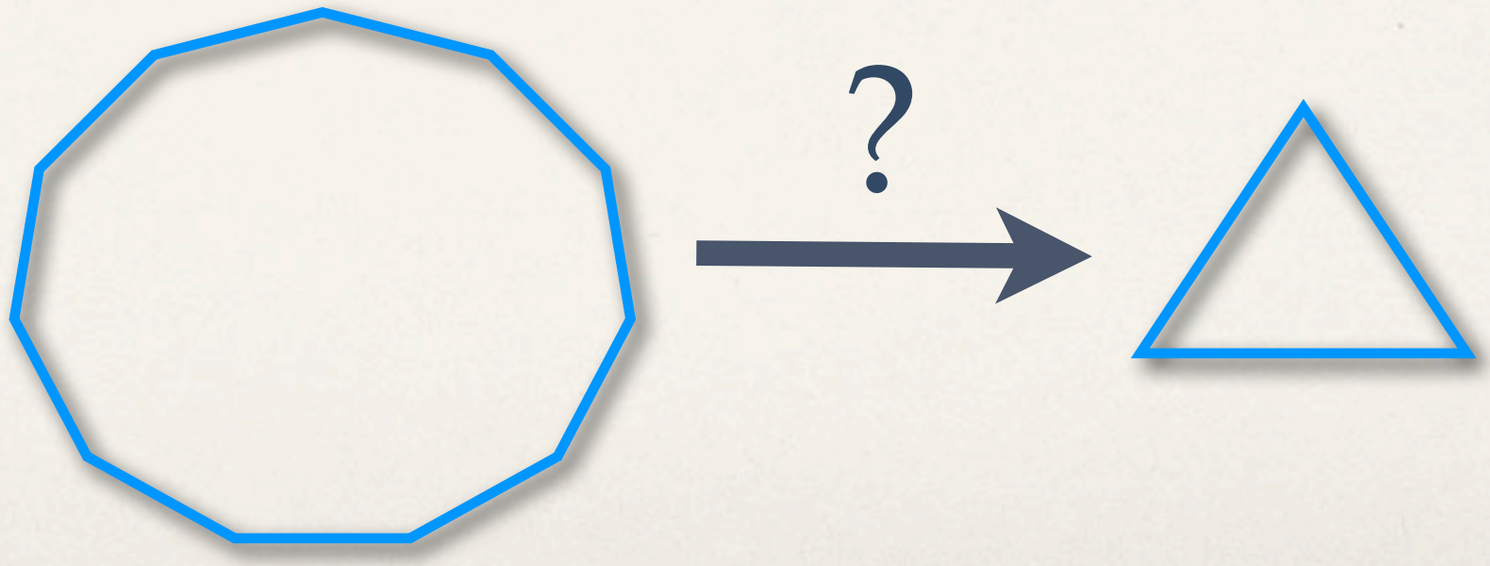

An SVM with an Exponentially Long Solution Path

- **Technical difficulties:**
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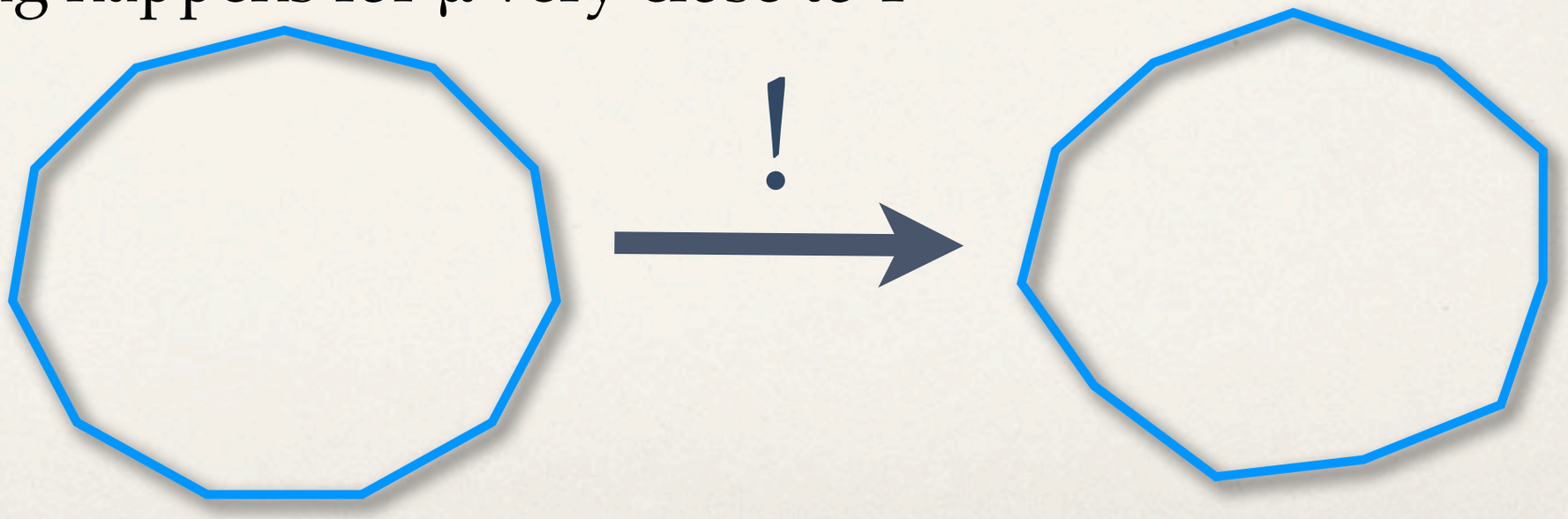
  - Solution: make line segment ——— so long that everything happens for μ very close to 1



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- The machine learning community is proficient in statistics, but not in geometry; it can be beneficial to look at some of their problems from a geometric viewpoint