Invariant Subspace Computation - A Geometric Approach

Pierre-Antoine Absil

PhD Defense

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Acknowledgements

Advisor:

Prof. R. Sepulchre
(Université de Liège)

Collaborations with:

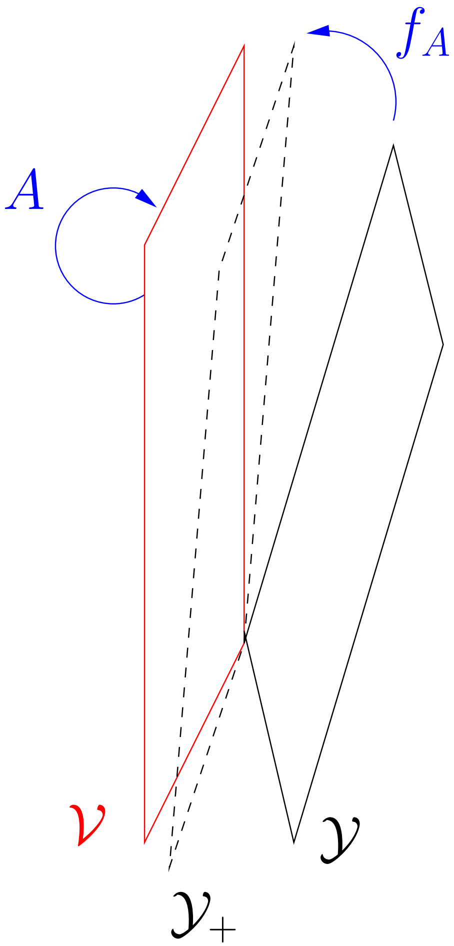
Prof. P. Van Dooren
(Université Catholique de Louvain)

Prof. R. Mahony
(Australian National University)

Outline

- Eigenspace computation: definitions.
- Eigenspace computation: an application.
- Geometric approach to eigenspace computation.
- New numerical algorithms:
  - Newton methods.
  - Shifted inverse iterations.
  - Global behaviour and improvements.

Topic: Refining estimates of eigenspaces



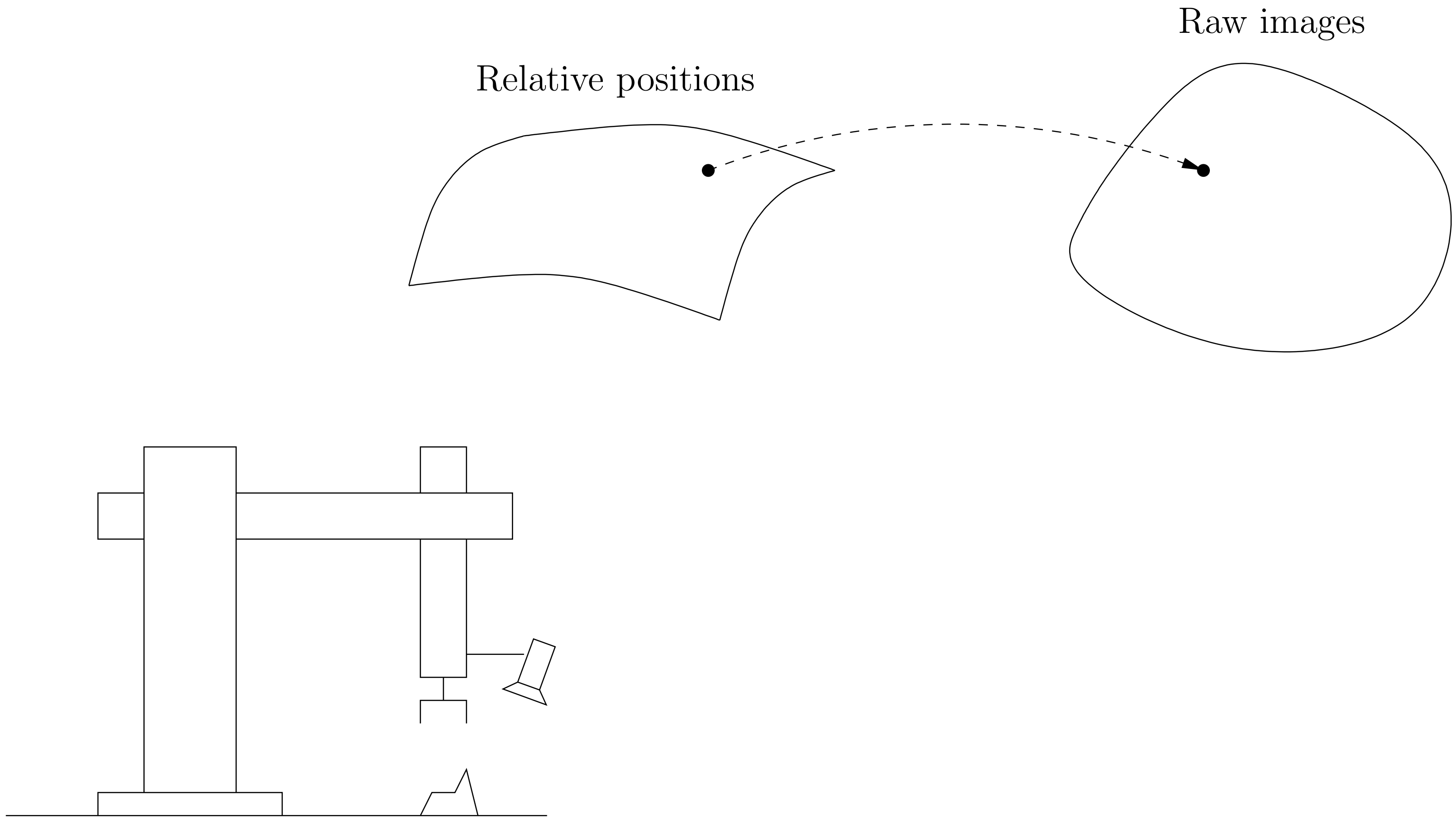
Data:

- n-by-n matrix A
- p-dimensional subspace $\mathcal{Y}$, approx. of eigenspace $\mathcal{V}$.

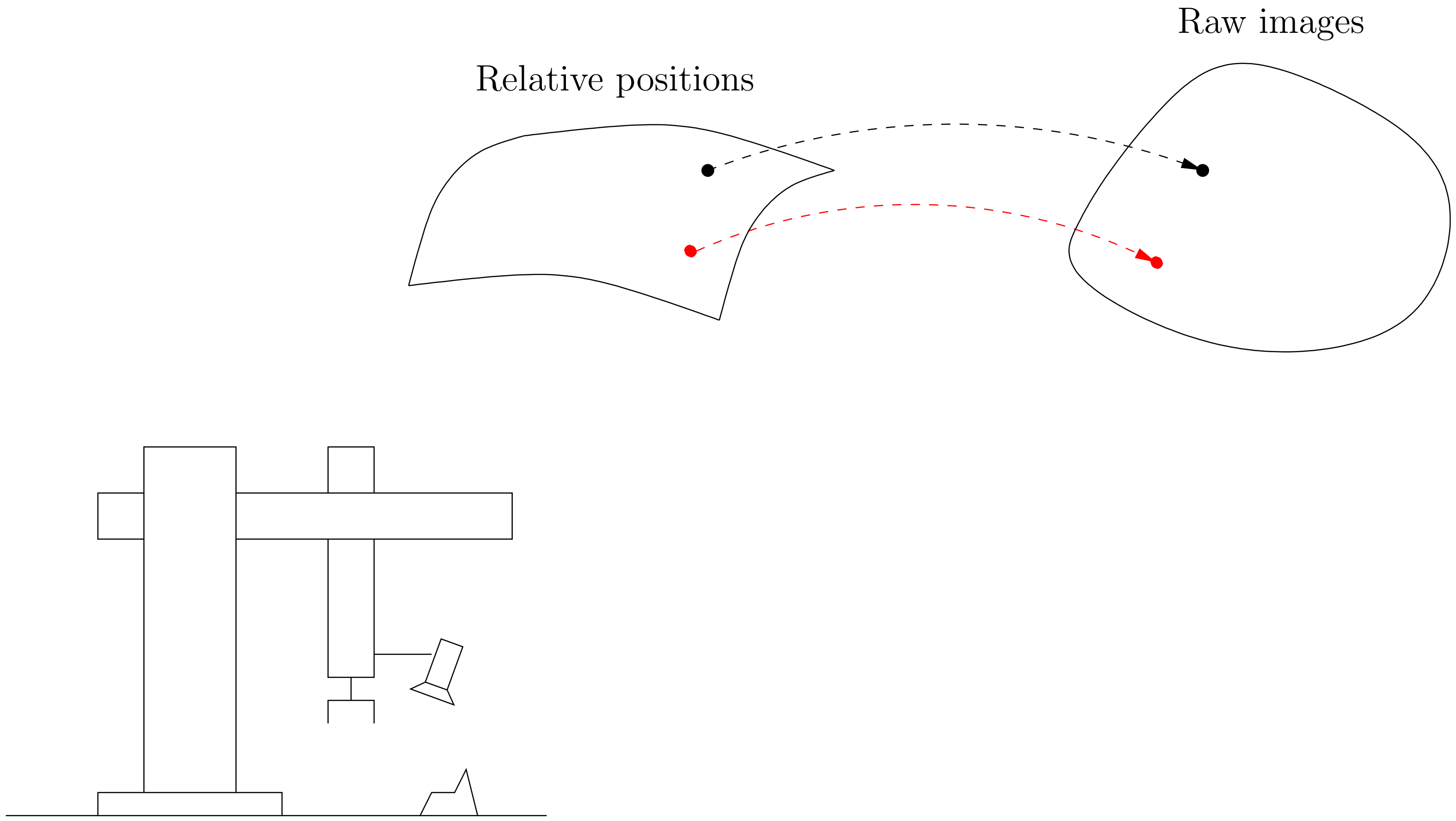
Task: compute better estimate of $\mathcal{V}$.

Definition of "eigenspace": $A\mathcal{V} \subseteq \mathcal{V}$.

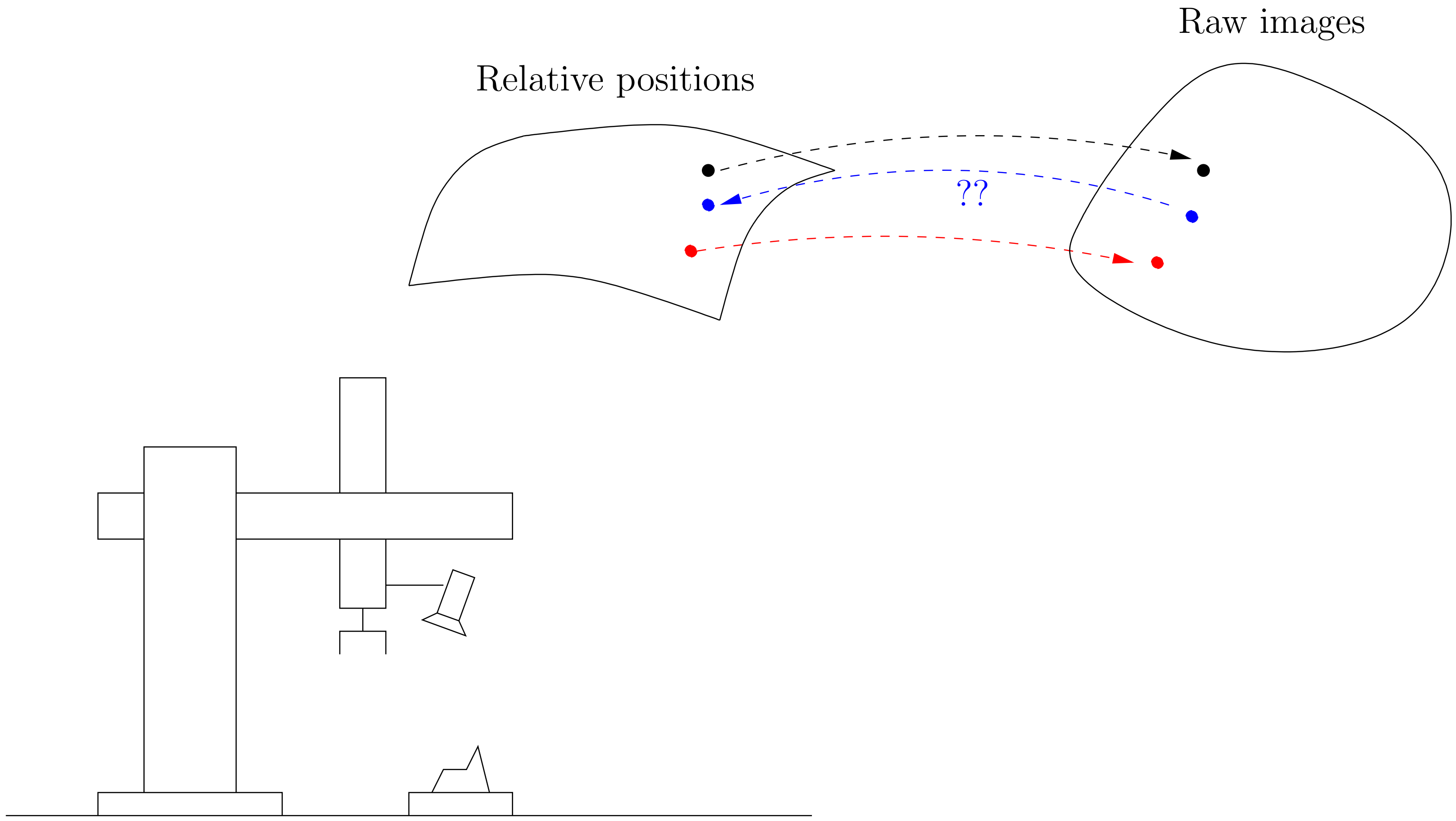
Application: visual positioning



Application: visual positioning



Application: visual positioning



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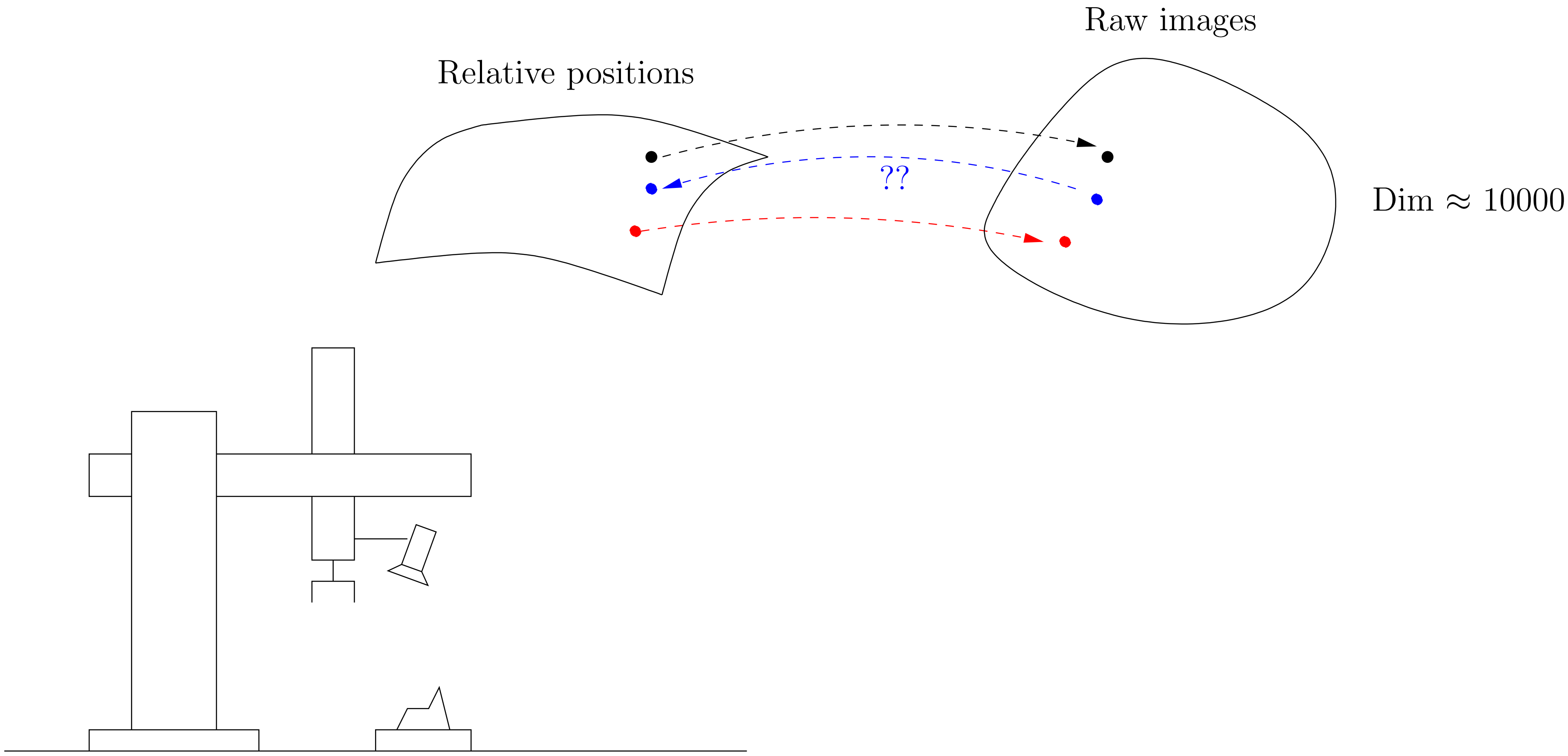
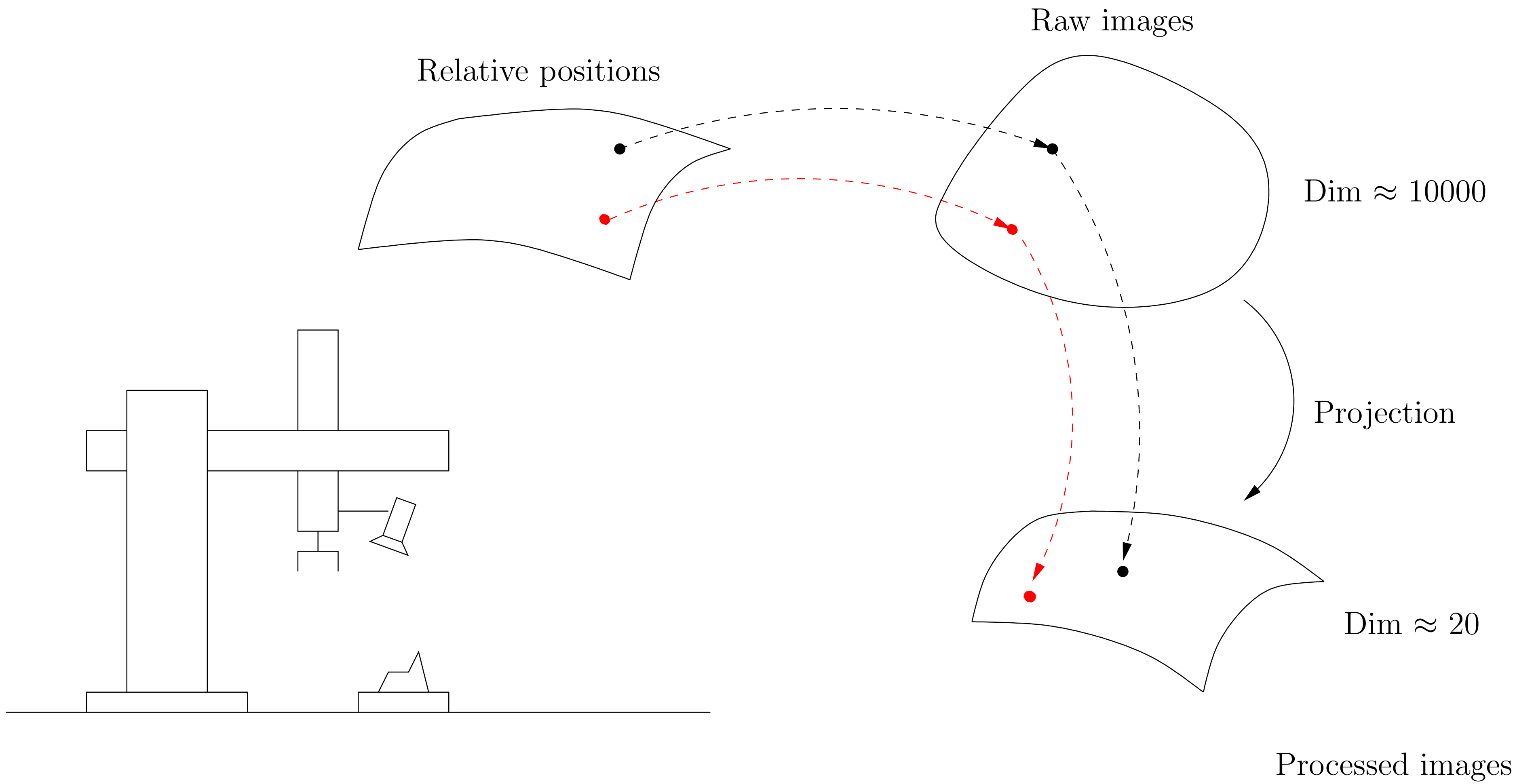


Application: visual positioning



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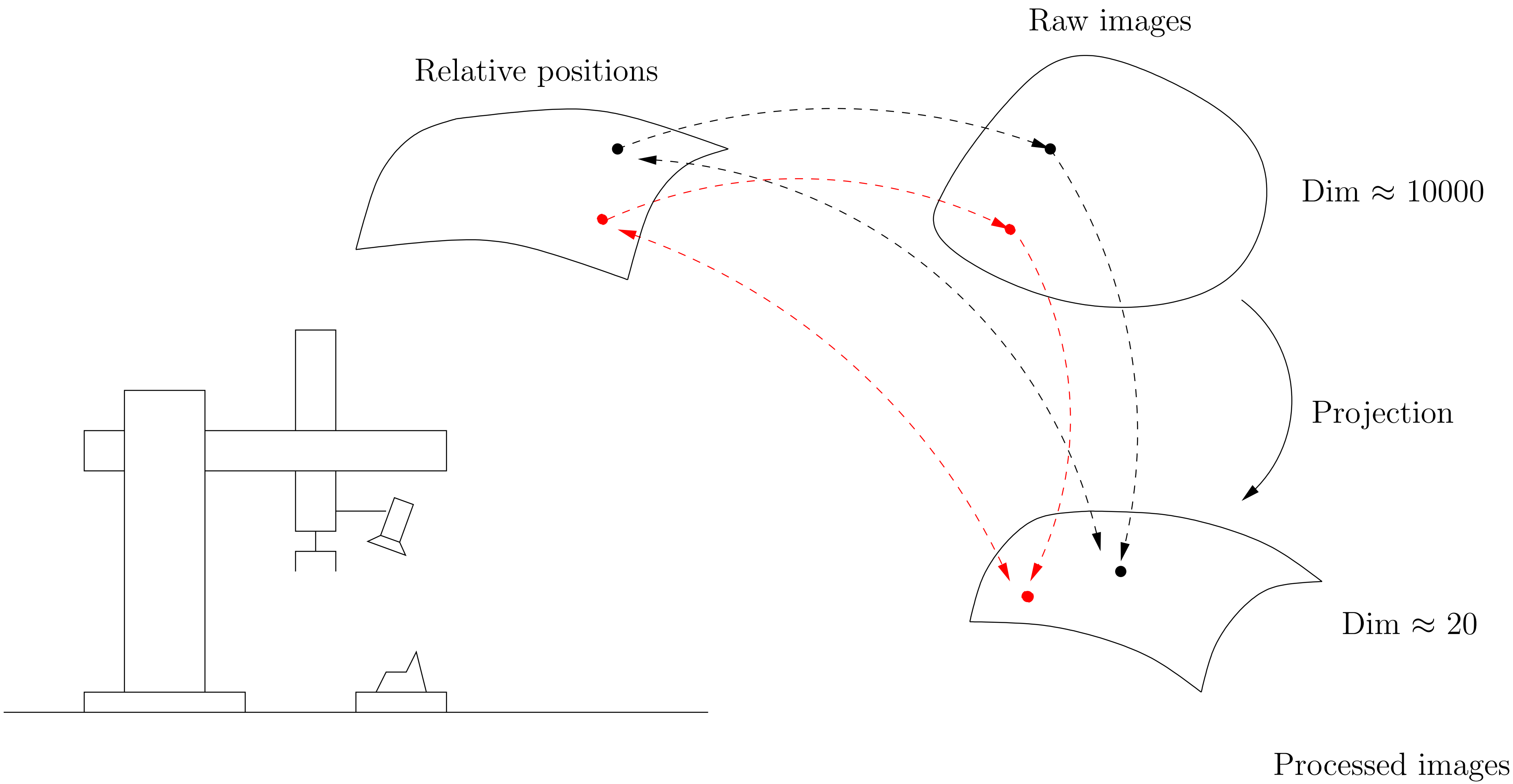

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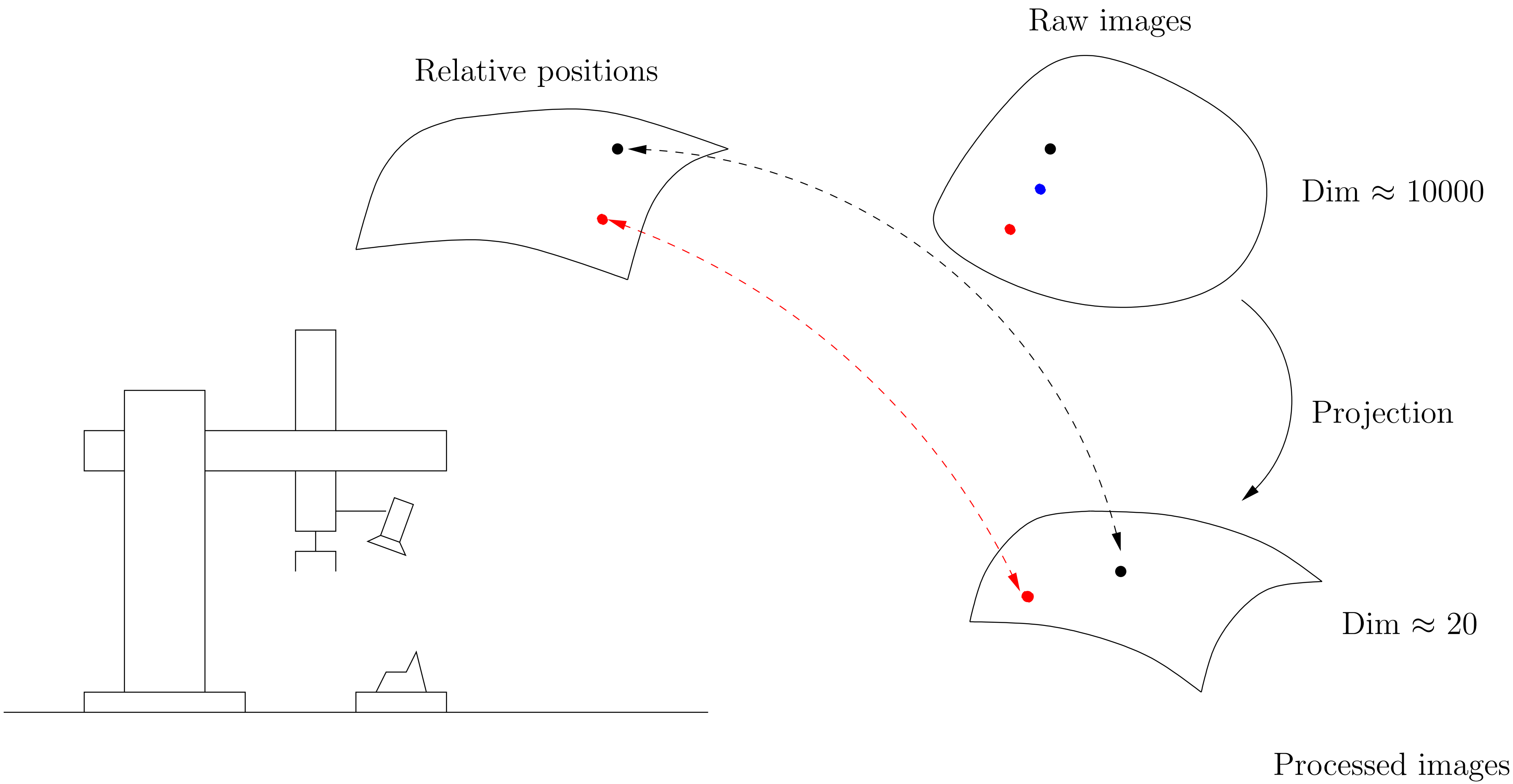

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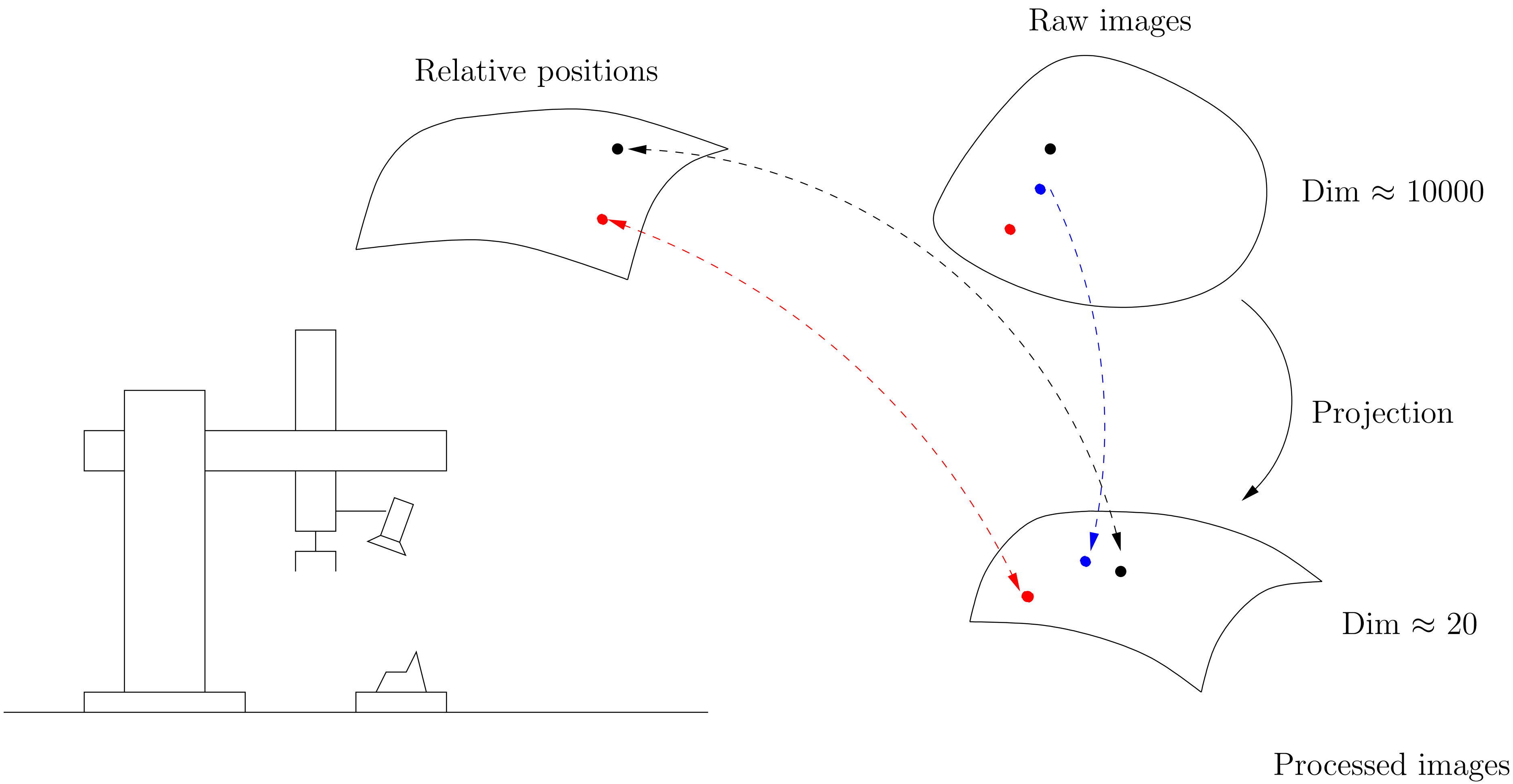
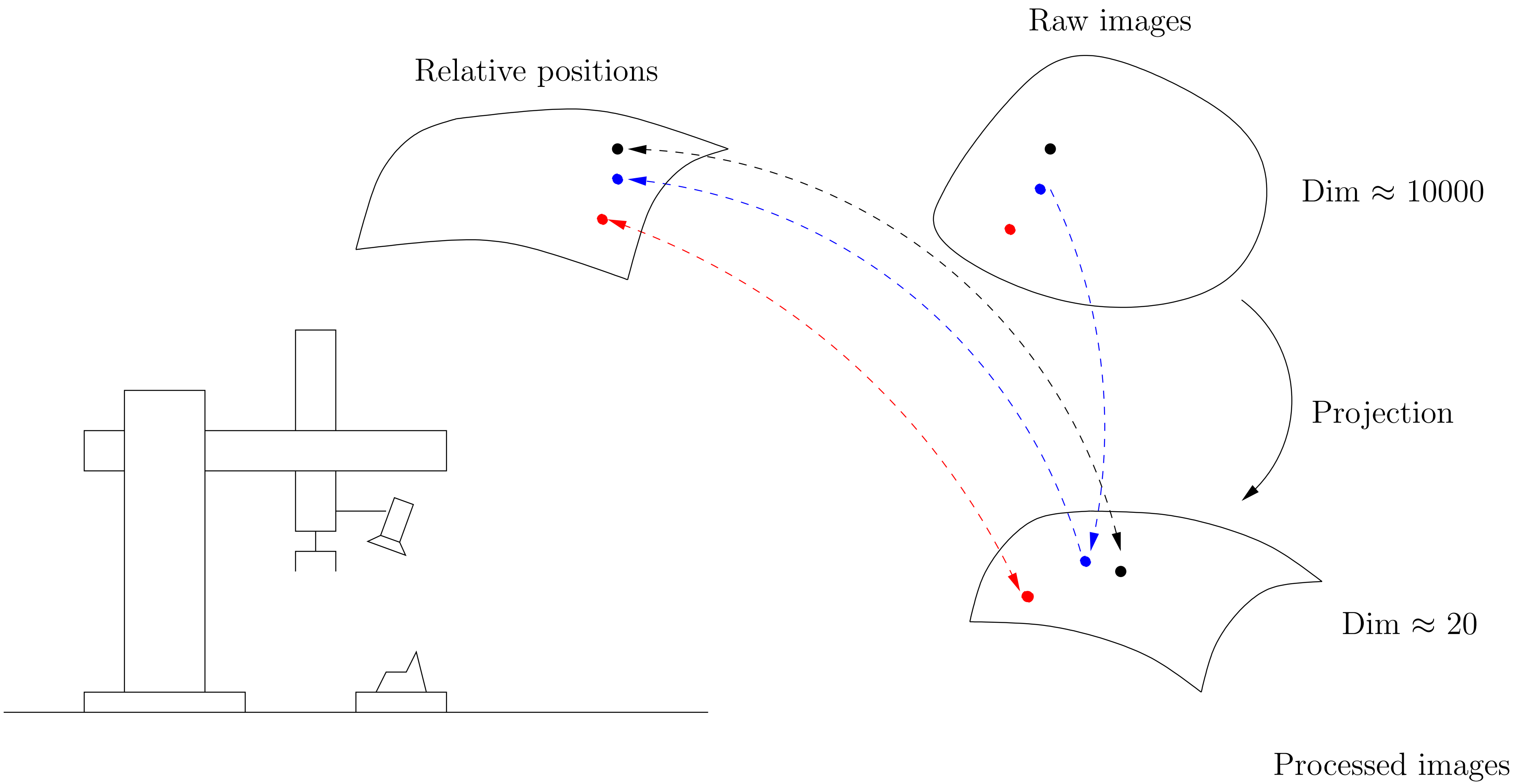
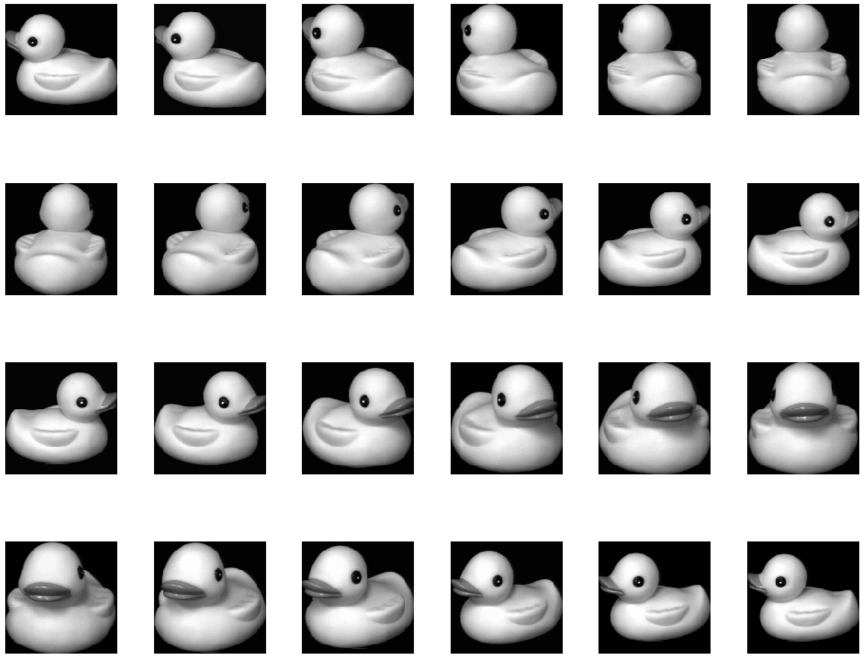


Application: visual positioning



Application: visual positioning

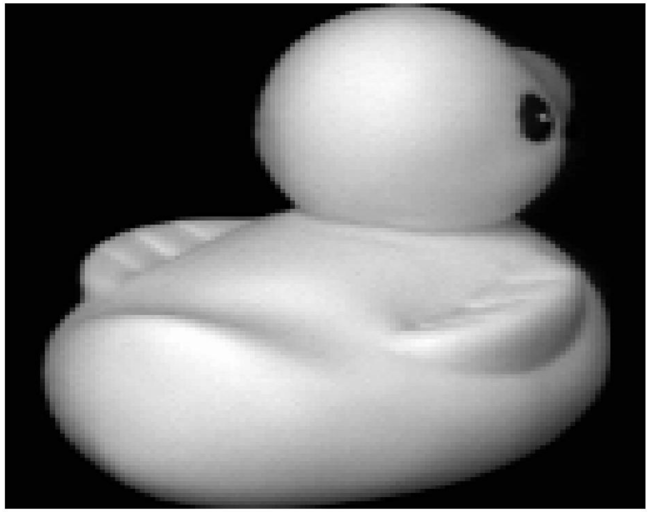
Learning...



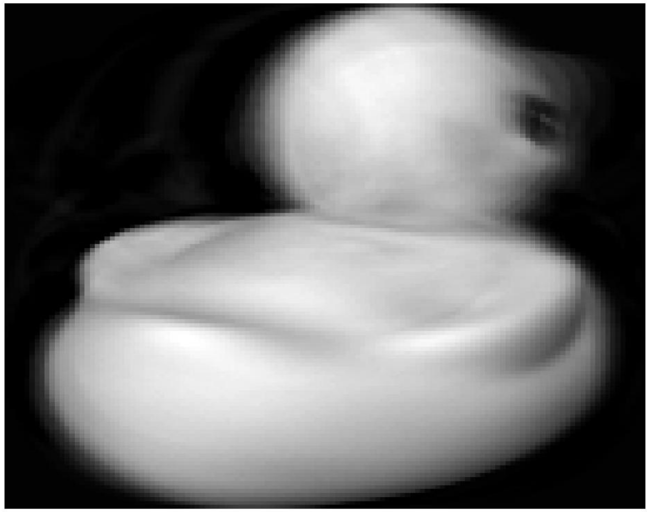
Compute covariance matrix and dominant eigenspace...

Application: visual positioning

Raw image

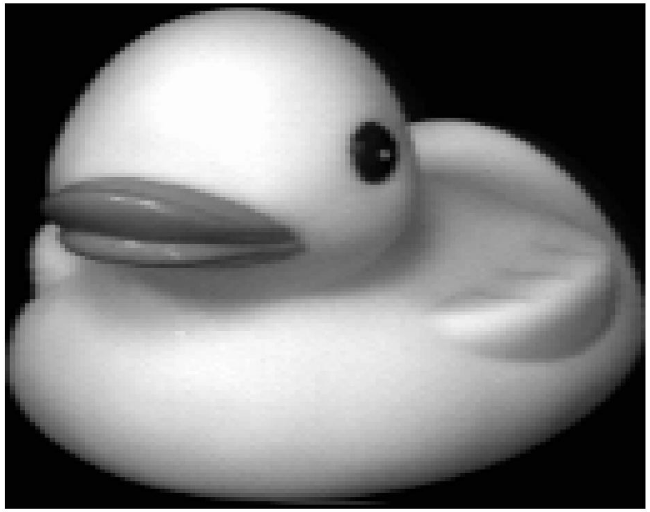


Projection onto eigenspace.

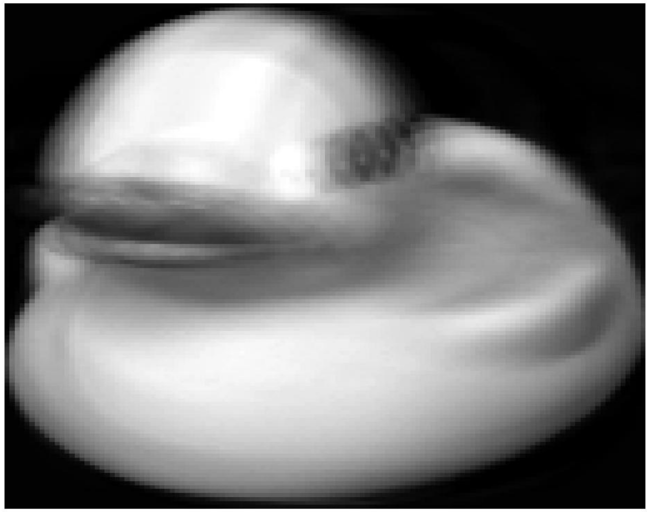


Application: visual positioning

Raw image



Projection onto eigenspace.



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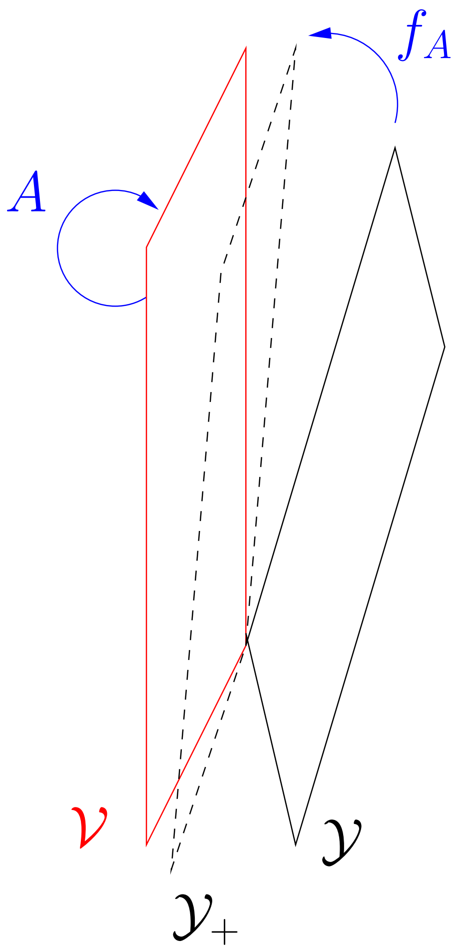
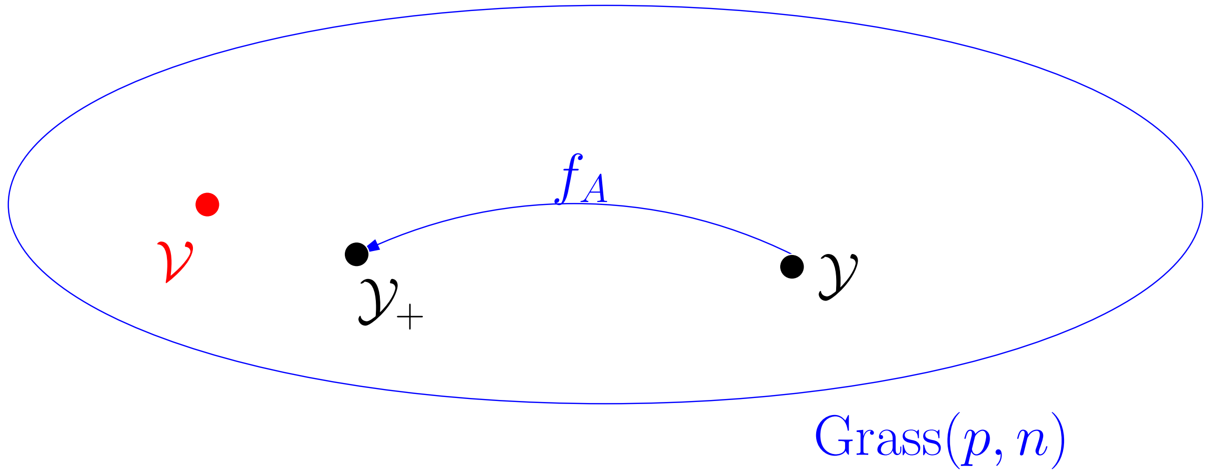
Refining estimates of eigenspaces

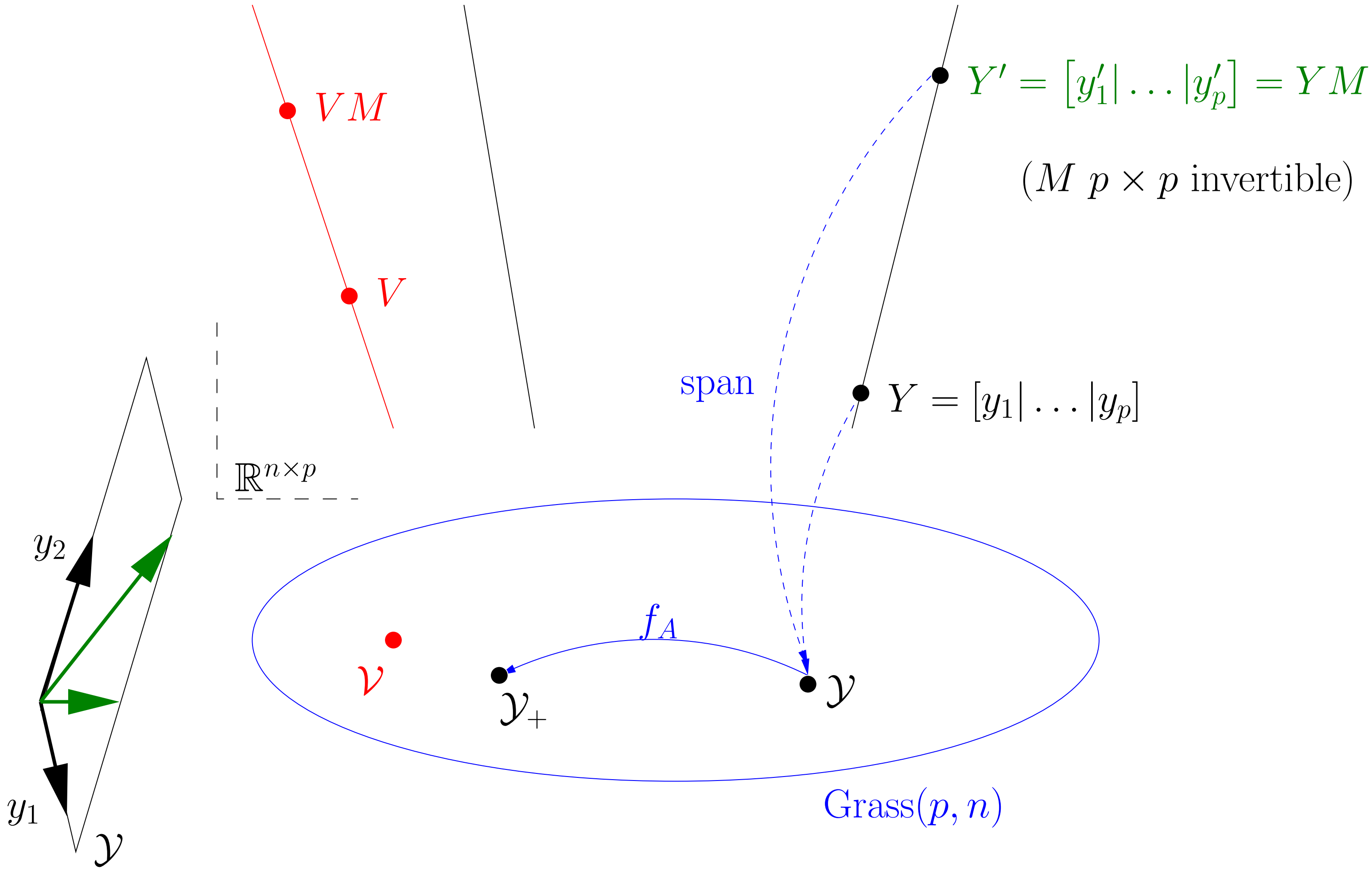




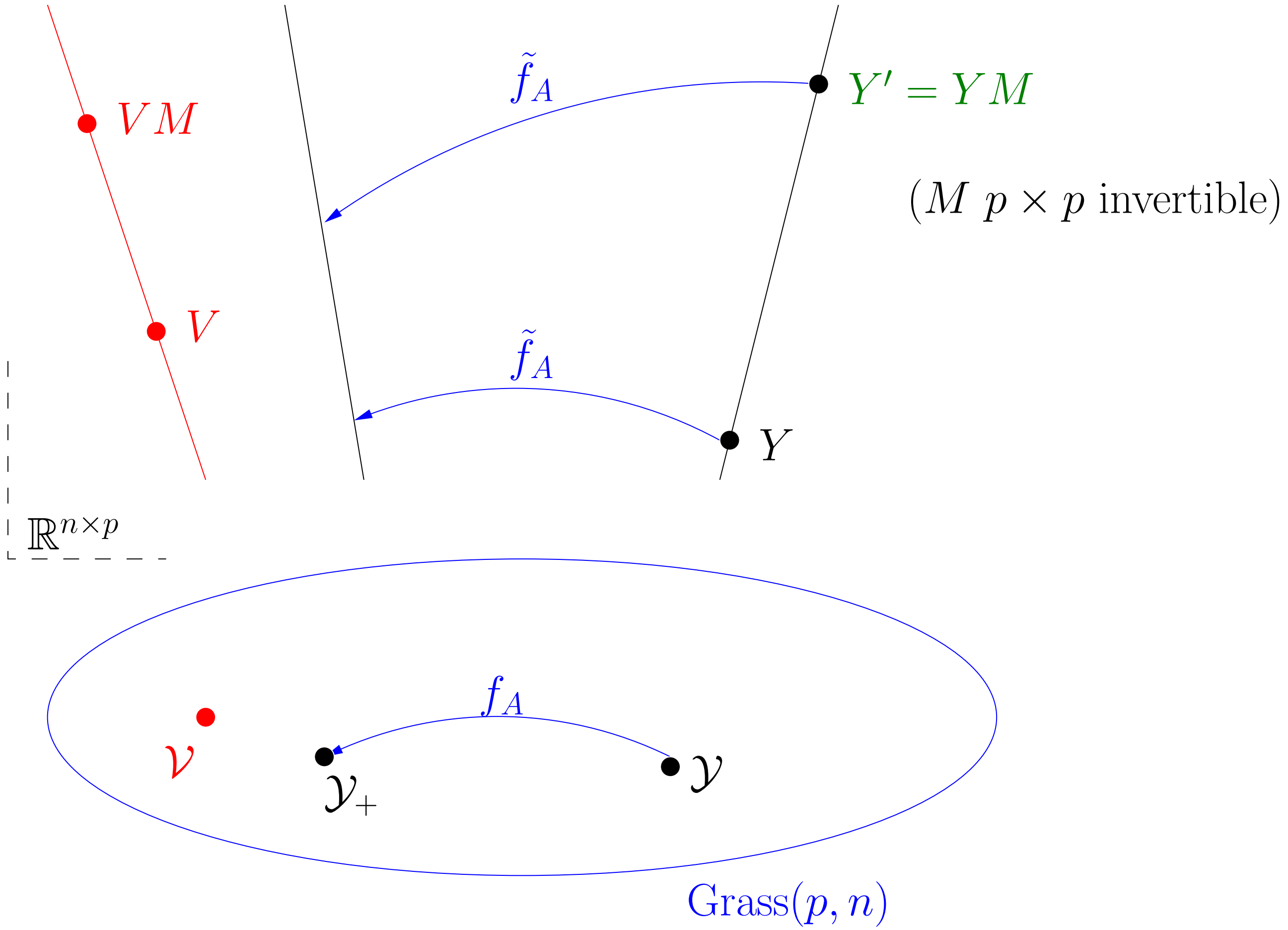
$p = \dim(\mathcal{V}) = \dim(\mathcal{Y}) = \dim(\mathcal{Y}_+)$.

Grass(p, n) (Grassmann manifold): the set of p-planes of $\mathbb{R}^n$.

Matrix representations



Iterations on the Grassmann manifold



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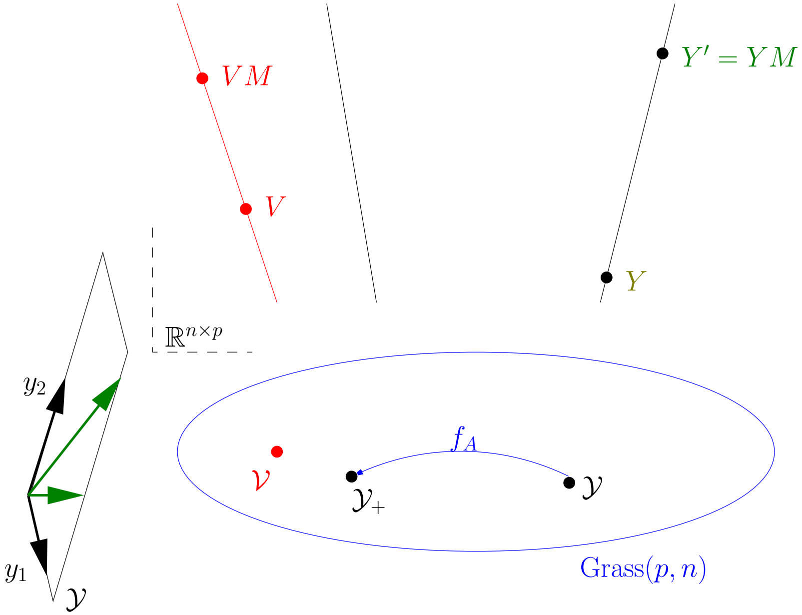
Newton method for eigenspace computation



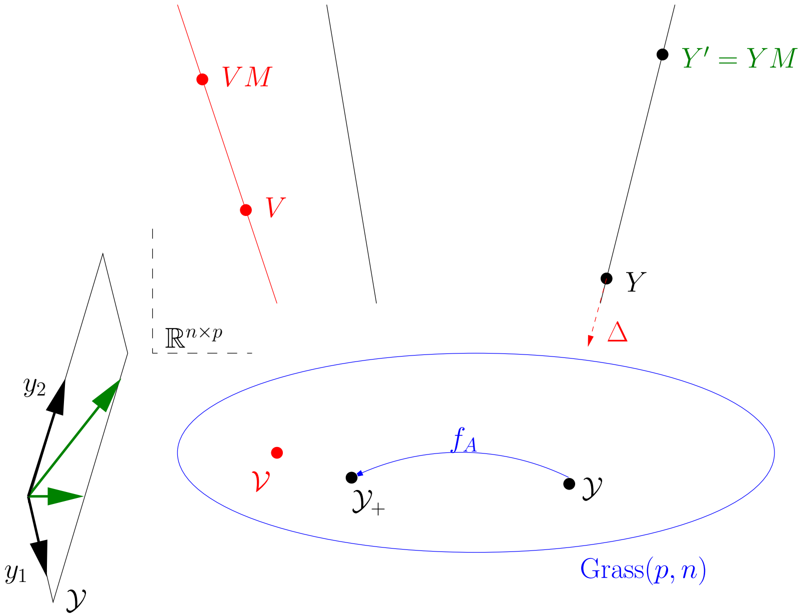
$F(Y) := \Pi_{Y_\perp} AY$, where
$\Pi_{Y_\perp} := I - Y(Y^T Y)^{-1} Y^T$.

Newton method in $\mathbb{R}^{n \times p}$:

$$F(Y) + \mathrm{D}F(Y)[\Delta] = 0$$

$$Y_+ = Y + \Delta$$

Newton method for eigenspace computation



$F(Y) := \Pi_{Y_\perp} AY$, where
$\Pi_{Y_\perp} := I - Y(Y^TY)^{-1}Y^T$.

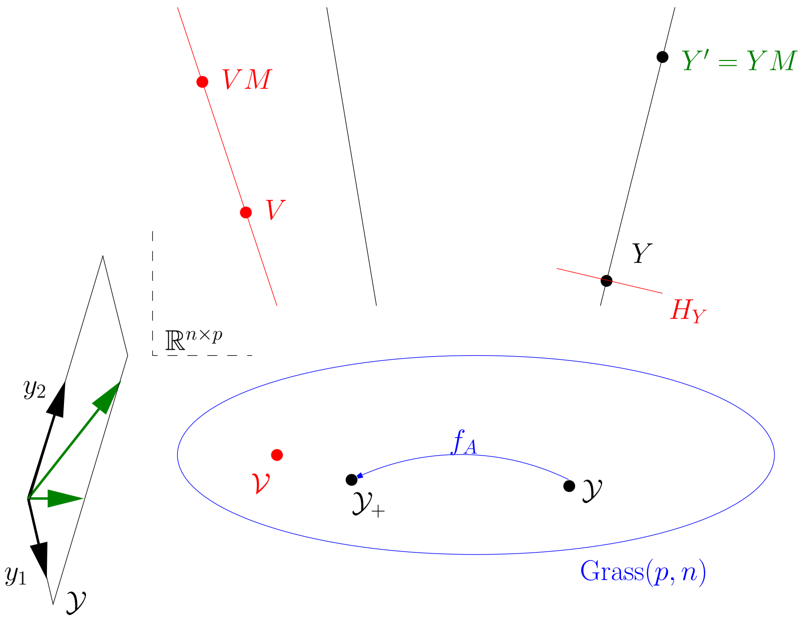
Newton method in $\mathbb{R}^{n\times p}$:

$$F(Y) + \mathrm{D}F(Y)[\Delta] = 0$$

$$Y_+ = Y + \Delta$$

Result: $\Delta = -Y$,
hence $Y_+ = 0$.

Newton method – Horizontal update



$F(Y) := \Pi_{Y_\perp} AY$, where
$\Pi_{Y_\perp} := I - Y(Y^TY)^{-1}Y^T$.

Newton method with constrained update:

$$\begin{cases} F(Y) + \mathrm{D}F(Y)[\Delta] = 0 \\ Y^T\Delta = 0 \end{cases}$$

Overdetermined system!

Newton method - Relaxations

Overdetermined system:

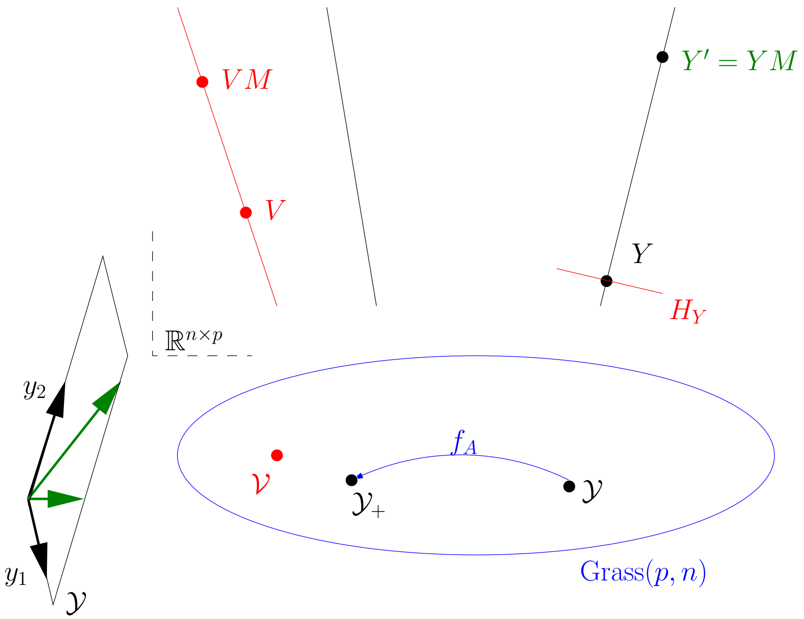
$$\begin{cases} F(Y) + \mathrm{D}F(Y)[\Delta] = 0 \\ Y^T\Delta = 0 \end{cases}$$

Two remedies:

- $$\Delta = \arg\min_{Y^T\Delta=0} \|F(Y) + \mathrm{D}F(Y)[\Delta]\|^2 = 0$$

- $$\begin{cases} \Pi_{Y_\perp}(F(Y) + \mathrm{D}F(Y)[\Delta]) = 0 \\ Y^T\Delta = 0 \end{cases}$$

Newton method – Riemannian interpretation



$$F(Y) := \Pi_{Y_\perp} AY$$

$$\begin{cases} \Pi_{Y_\perp}(F(Y) + \mathrm{D}F(Y)[\Delta]) = 0 \\ Y^T\Delta = 0 \end{cases}$$

$$Y_+ = Y + \Delta.$$

Riemannian Newton method:

$$F(Y) + \nabla_\Delta F(Y) = 0$$

$$Y_+ = \mathrm{Exp}(\Delta)$$

Newton method for eigenspace computation

Iteration mapping: $\mathrm{Grass}(p,n) \ni \mathcal{Y} \mapsto \mathcal{Y}_+ \in \mathrm{Grass}(p,n)$ defined by

1. Pick a basis $Y \in \mathbb{R}^{n\times p}$ that spans $\mathcal{Y}$ and solve the equation

$$\Pi A \Pi \Delta - \Delta (Y^T Y)^{-1} Y^T A Y = -\Pi A Y \tag{1}$$

under the constraint $Y^T \Delta = 0$, where $\Pi := I - Y(Y^T Y)^{-1} Y^T$.

2. Perform the update

$$\mathcal{Y}_+ = \mathrm{span}(Y + \Delta). \tag{2}$$

Newton method – Related work

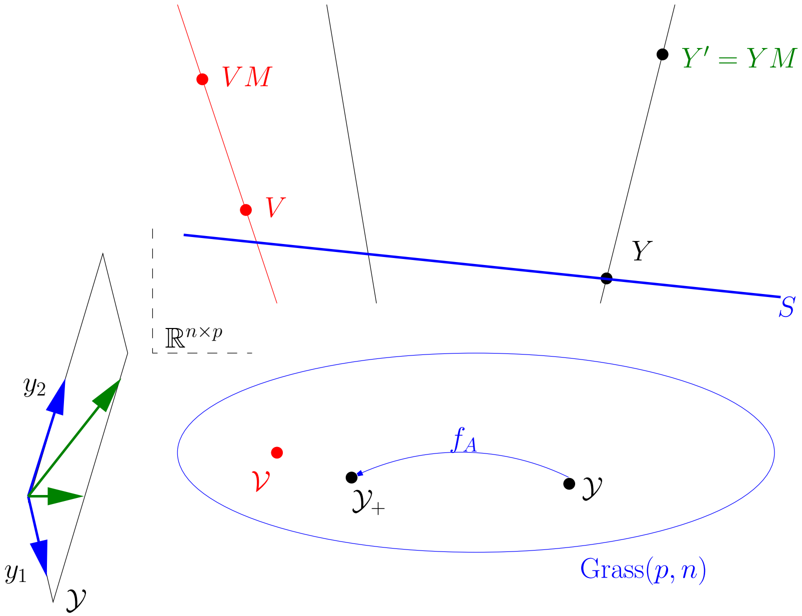
Previous work:

- Stewart [Ste73], Dongarra, Moler and Wilkinson [DMW83], Chatelin [Cha84], Demmel [Dem87].
- Lösche, Schwetlick and Timmerman [LST98].
- Edelman, Arias and Smith [EAS98].
- Lundström and Elden [LE02].

New results (PAA, Mahony, Sepulchre [AMS02]):

- Iteration converges locally quadratically (even when $A \neq A^T$).
- Convergence is locally cubic iff $A^T\mathcal{V} \subseteq \mathcal{V}$.

Newton method – Cross sections

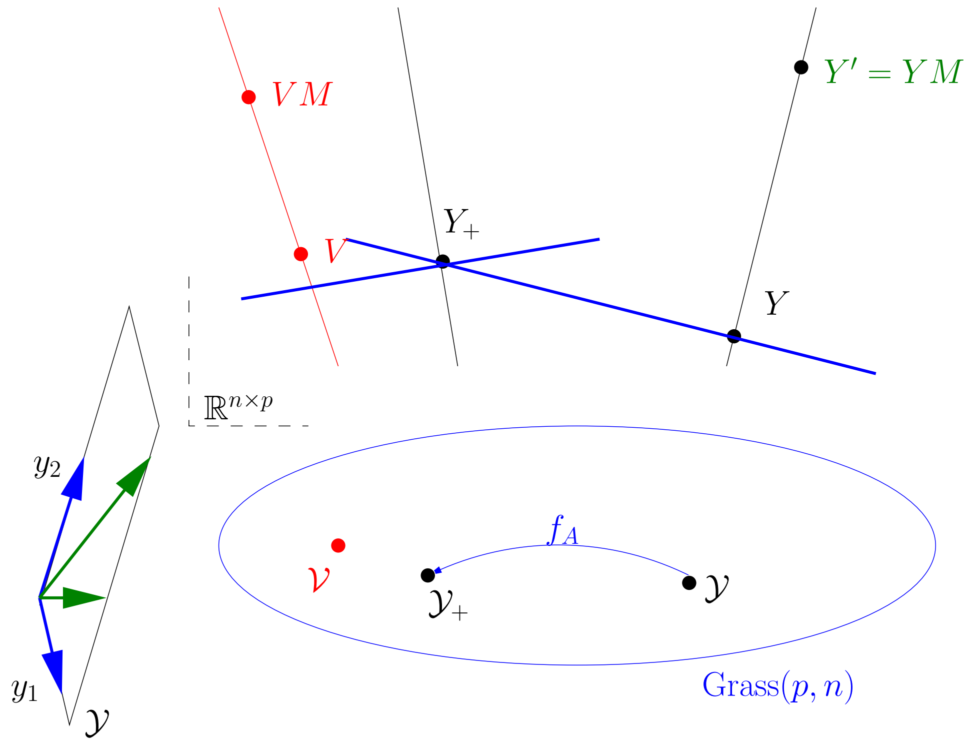


Parameterize S:
$Y = W + W_\perp K$.
Then $\Pi A Y = 0$ becomes a quadratic matrix equation

$$A_{22}K - KA_{11} + A_{21} - KA_{12}K = 0$$

where $A_{11} = W^T A W$, $A_{12} = W^T A W_\perp$, $A_{21} = W_\perp^T A W$ and $A_{22} = W_\perp^T A W_\perp$.

Newton method – Adaptive cross section



Advantage: if $A = A^T$, convergence is cubic, instead of quadratic in the fixed cross section case.

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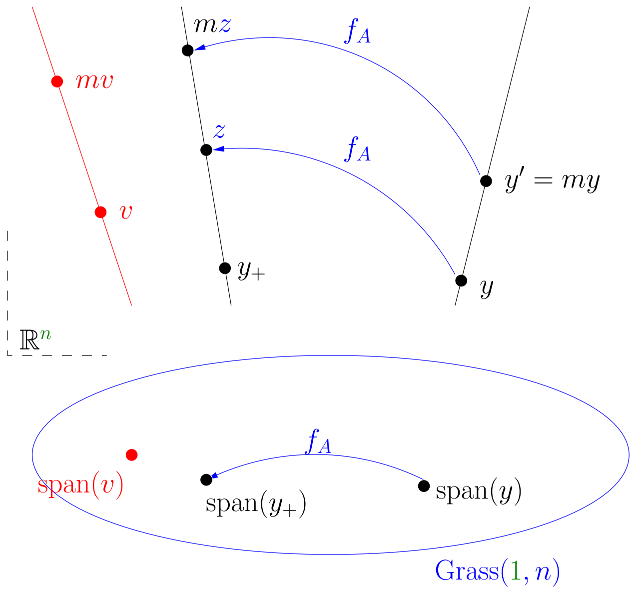
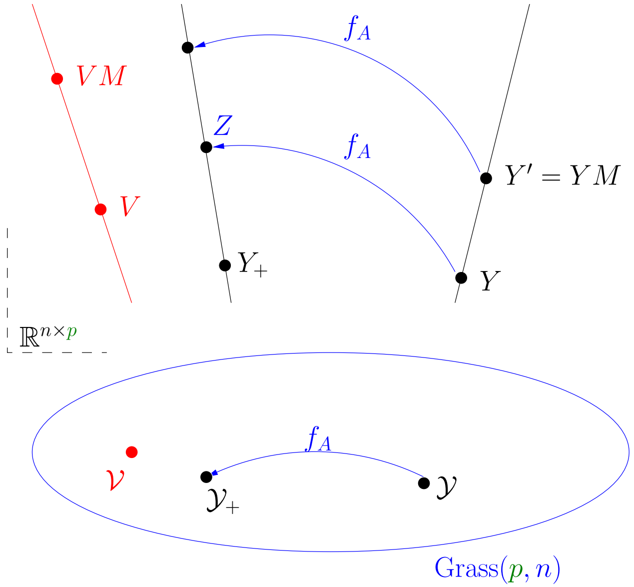
Rayleigh Quotient Iteration – Case $p = 1$



$$(A - \rho(y)I)z = y$$
$$\rho(y) := (y^T Ay)/(y^T y).$$

Local cubic convergence to eigendirections of $A = A^T$.

Rayleigh Quotient Iteration – From $p = 1$ to $p \geq 1$



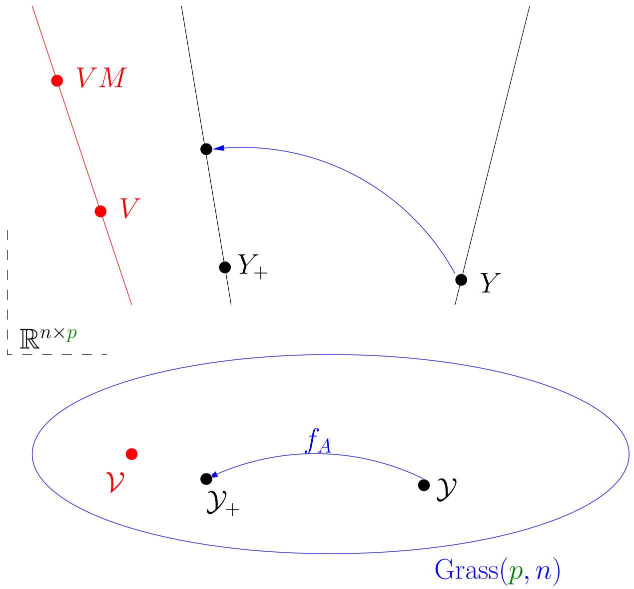
$$(A - \rho(y)I)z = y$$
$$\rho(y) := (y^T Ay)/(y^T y).$$

$$\xrightarrow{p>1} ??$$

Want:

- Well defined on Grass(p, n).
- Reduces to RQI when $p = 1$.
- Local cubic convergence.

Rayleigh Quotient Iteration – Case $p \geq 1$



Classical Rayleigh Quotient Iteration ($p = 1$):

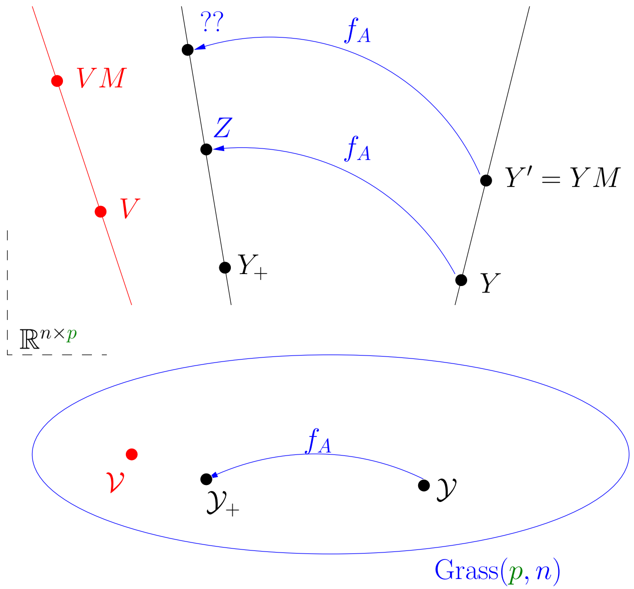
$(A - \rho(y)I)z = y$

$\rho(y) := (y^T Ay)/(y^T y)$.

Generalized iteration ($p \geq 1$):

$AZ - Z(Y^T Y)^{-1} Y^T AY = Y$.

Rayleigh Quotient Iteration – From $p = 1$ to $p \geq 1$



$$(A - \rho(y)I)z = y$$
$$\rho(y) := (y^T AY)/(y^T y).$$

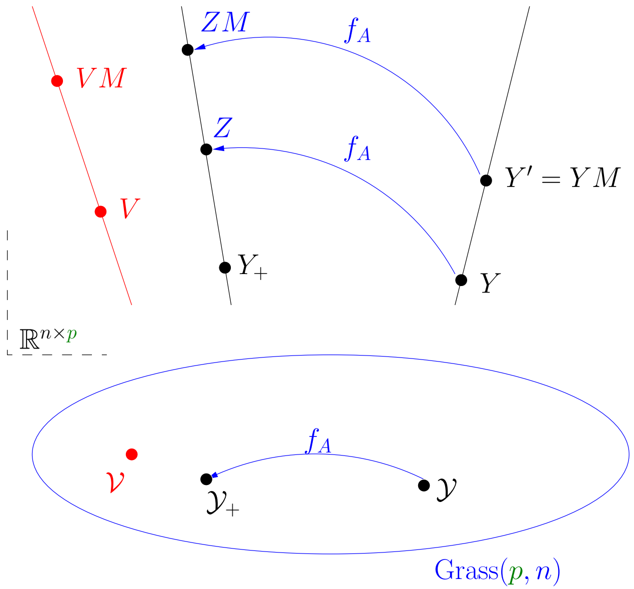
Generalized iteration:

$$AZ - Z(Y^T Y)^{-1} Y^T AY = Y.$$

Want:

- $\rightarrow$ Well defined on Grass(p, n).
- $\rightarrow$ Reduces to RQI when $p = 1$.
- $\rightarrow$ Local cubic convergence.

Rayleigh Quotient Iteration – From $p = 1$ to $p \geq 1$



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Want:

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- $\longrightarrow$ Reduces to RQI when $p = 1$.
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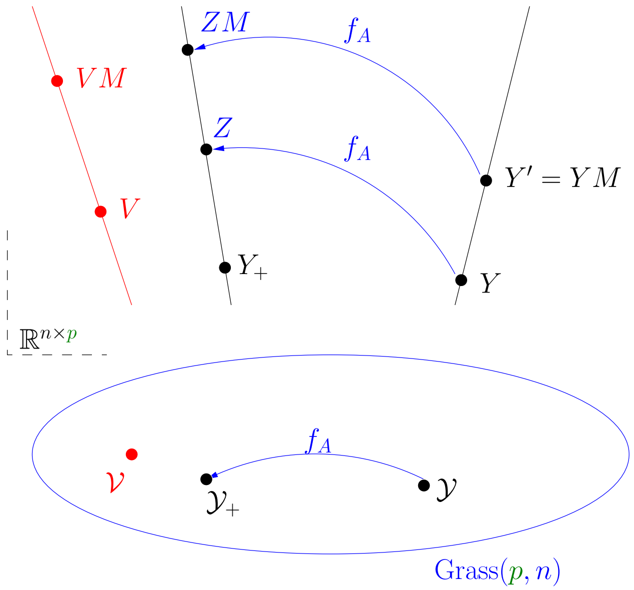
Rayleigh Quotient Iteration – From $p = 1$ to $p \geq 1$



$$(A - \rho(y)I)z = y$$

$$\rho(y) := (y^T AY)/(y^T y).$$

Generalized iteration:

$$AZ - Z(Y^T Y)^{-1} Y^T AY = Y.$$

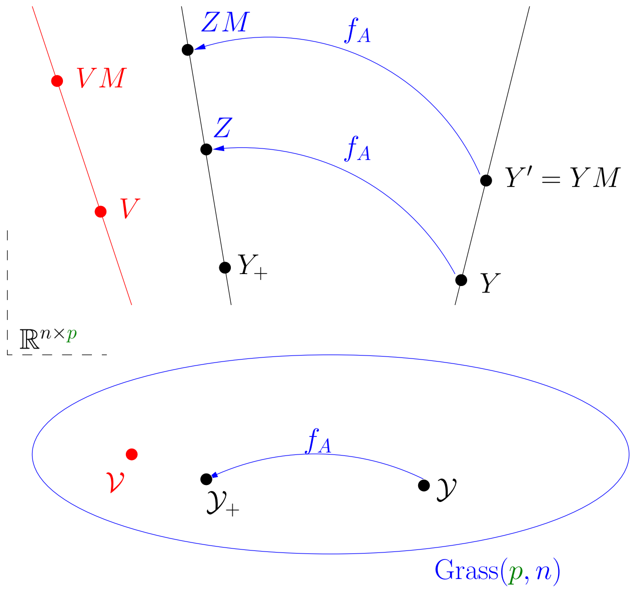
Want:

→ Well defined on Grass(p, n).

→ Reduces to RQI when $p = 1$.

→ Local cubic convergence.

Rayleigh Quotient Iteration – From $p = 1$ to $p \geq 1$



$$(A - \rho(y)I)z = y$$
$$\rho(y) := (y^T AY)/(y^T y).$$

Generalized iteration:

$$AZ - Z(Y^TY)^{-1}Y^TAY = Y.$$

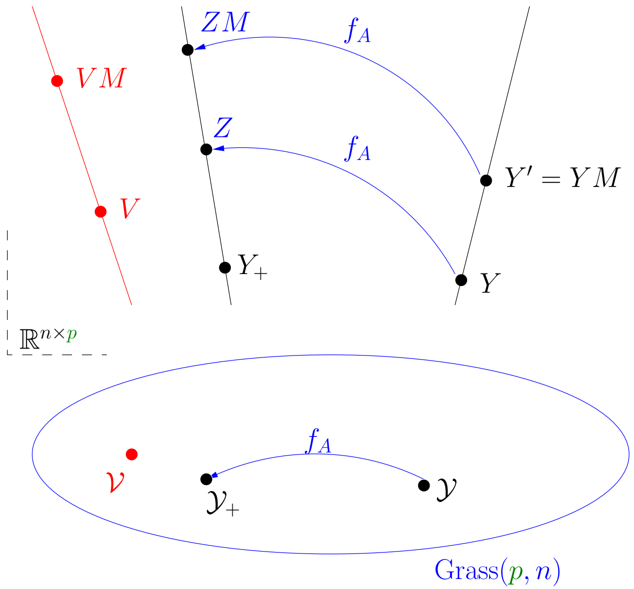
Want:

→ Well defined on Grass(p, n).

→ Reduces to RQI when $p = 1$.

→ Local cubic convergence.

Rayleigh Quotient Iteration – From $p = 1$ to $p \geq 1$



$$(A - \rho(y)I)z = y$$

$$\rho(y) := (y^T AY)/(y^T y).$$

Generalized iteration:

$$AZ - Z(Y^TY)^{-1}Y^TAY = Y.$$

Want:

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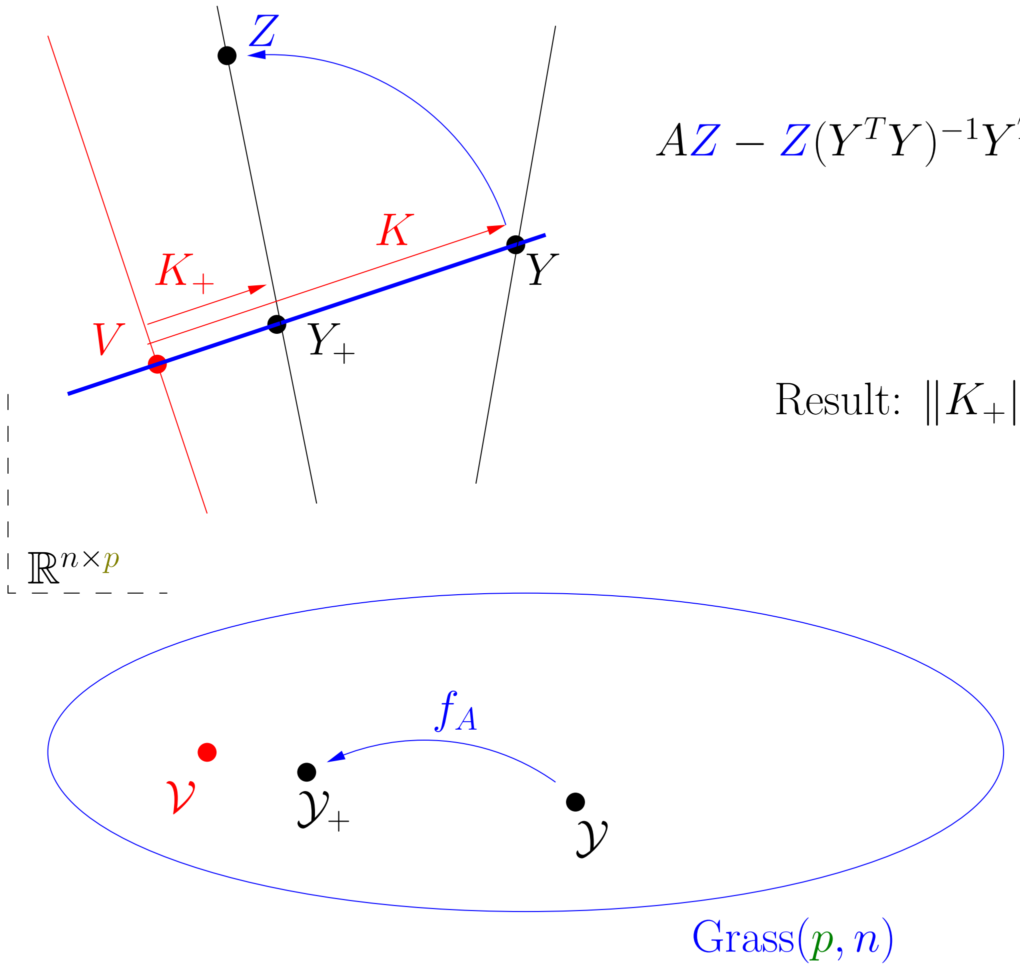
→ Local cubic convergence.

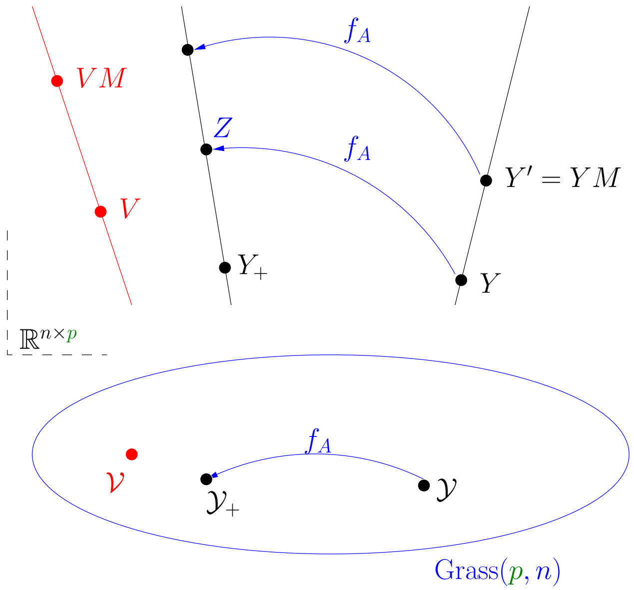
Rayleigh Quotient Iteration – Local Convergence



$$AZ - Z(Y^TY)^{-1}Y^TAY = Y$$

Result: $\|K_+\| \leq c\|K\|^3$

Rayleigh Quotient Iteration – From $p = 1$ to $p \geq 1$



$$(A - \rho(y)I)z = y$$
$$\rho(y) := (y^T AY)/(y^T y).$$

Generalized iteration:

$$AZ - Z(Y^T Y)^{-1} Y^T AY = Y.$$

Want:

$\longrightarrow$ Well defined on Grass(p, n).

$\longrightarrow$ Reduces to RQI when $p = 1$.

$\longrightarrow$ Local cubic convergence.

Rayleigh Quotient Iteration – The matrix algorithm

Iteration mapping: $\mathrm{Grass}(p,n) \ni \mathcal{Y} \mapsto \mathcal{Y}_+ \in \mathrm{Grass}(p,n)$ defined by

1. Pick a basis $Y \in \mathbb{R}^{n\times p}$ that spans $\mathcal{Y}$.
2. Solve

$$AZ - Z(Y^TY)^{-1}Y^TAY = Y \tag{3}$$

for $Z \in \mathbb{R}^{n\times p}$.

3. Define $\mathcal{Y}_+$ as the span of Z.

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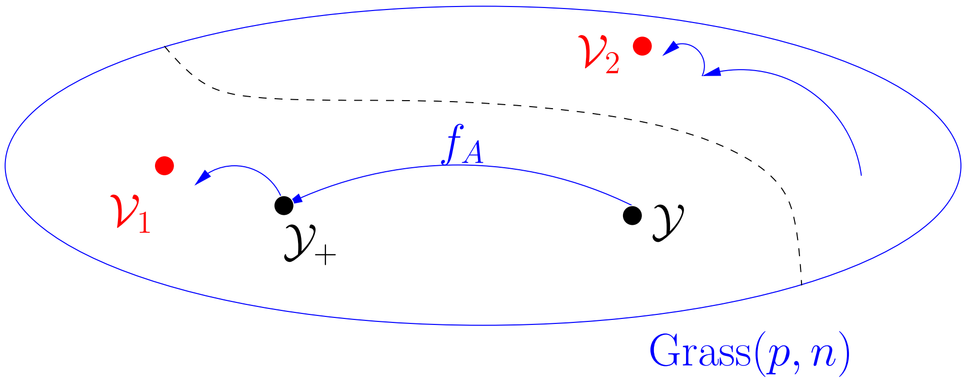
Global behaviour of iterative methods

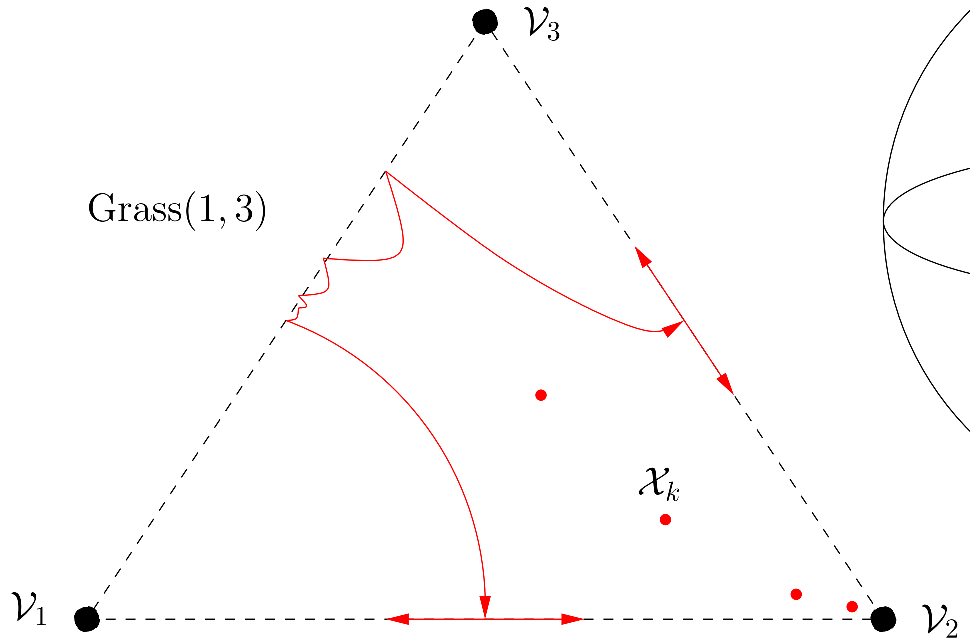


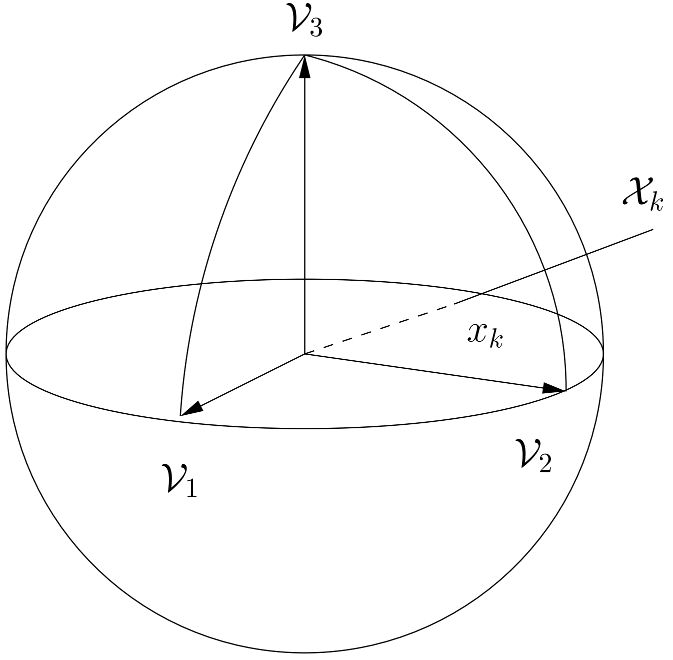
Study basins of attraction of eigenspaces.

Global behaviour for $p = 1$

When $p = 1$,

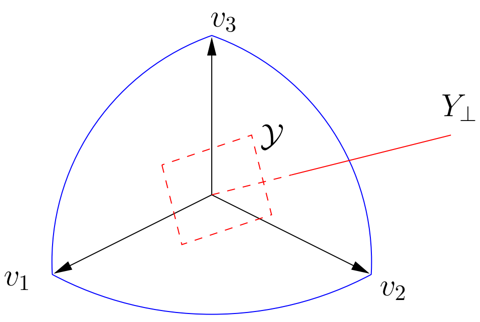
Riemannian Newton method $\equiv$ Rayleigh Quotient Iteration.

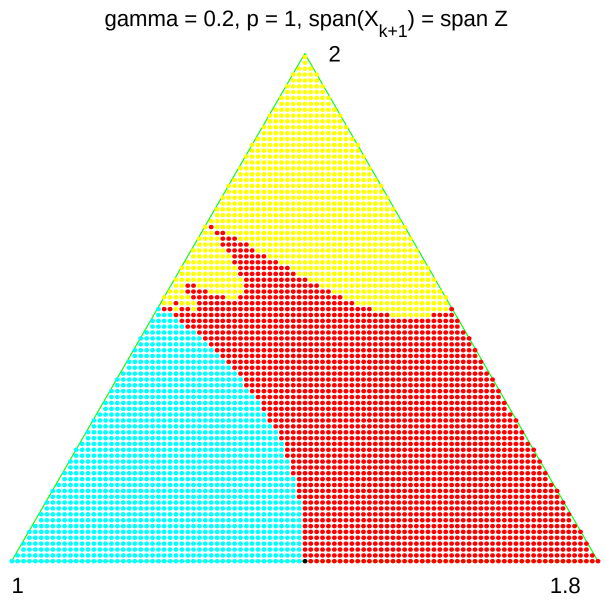


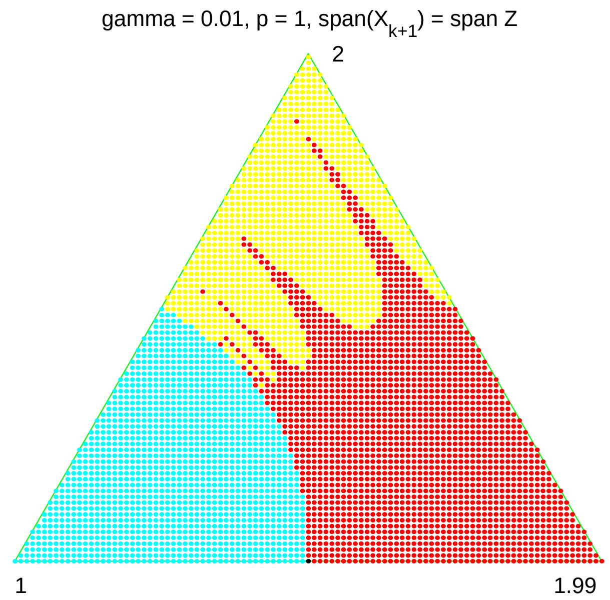


Reference: Batterson and Smillie [BS89].

Newton method – Global behaviour

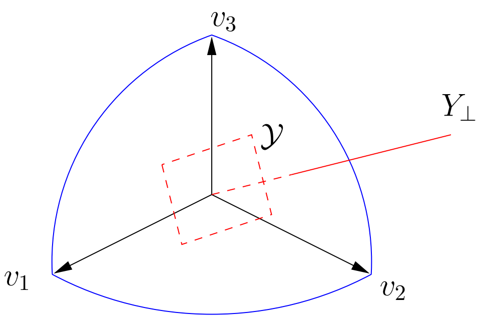


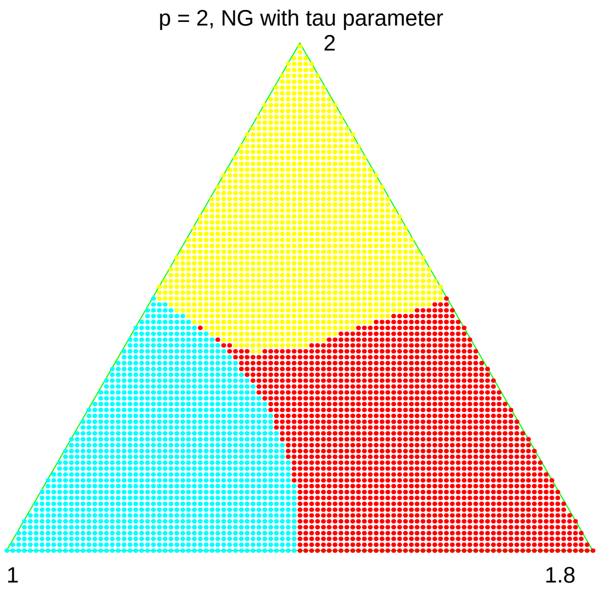


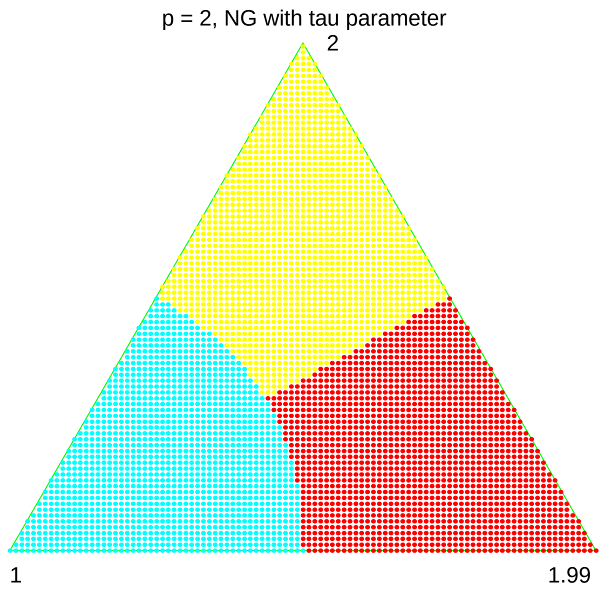


Basins may deteriorate when eigenvalues are clustered.

Newton method – Improved global behaviour







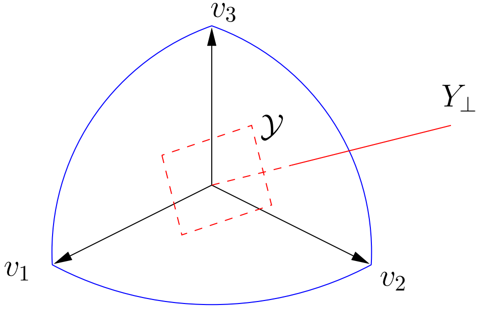
Remedy: modified Newton methods with large basins of attraction.

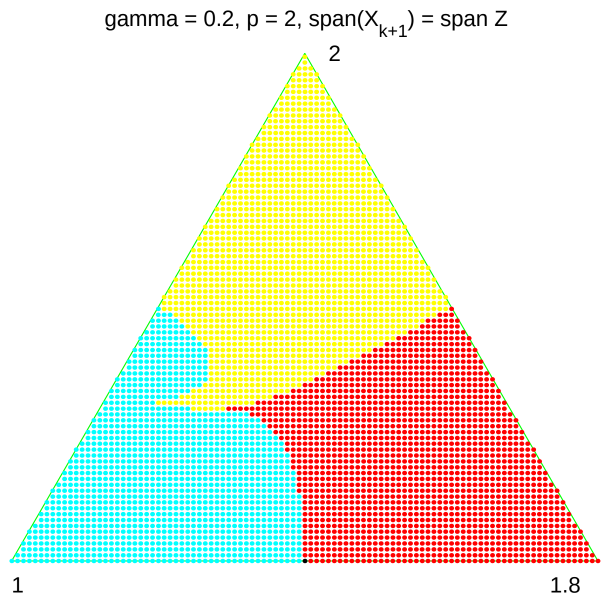
Rayleigh Quotient Iteration – Global behaviour ($p > 1$)

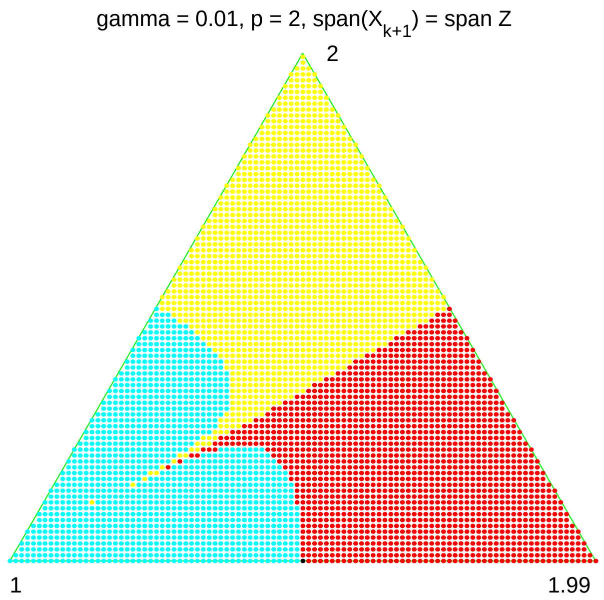
$$AZ - Z(Y^TY)^{-1}Y^TAY = Y, \; Y_+ = ZM$$

Theoretical results: ?

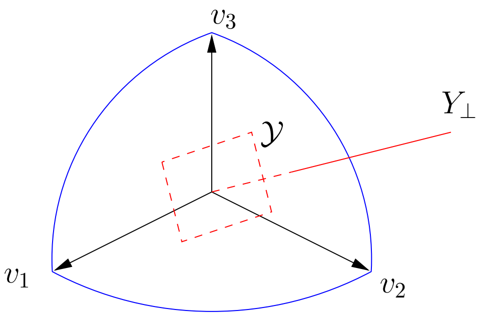
Experimental results:

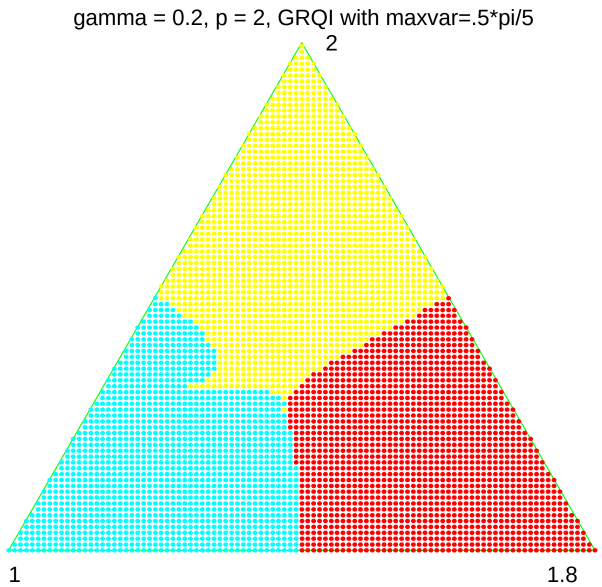


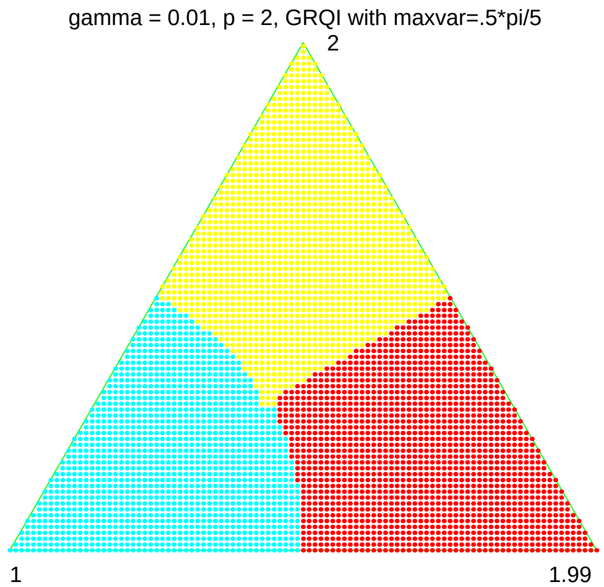




Rayleigh Quotient Iteration – Improved global behaviour ($p > 1$)







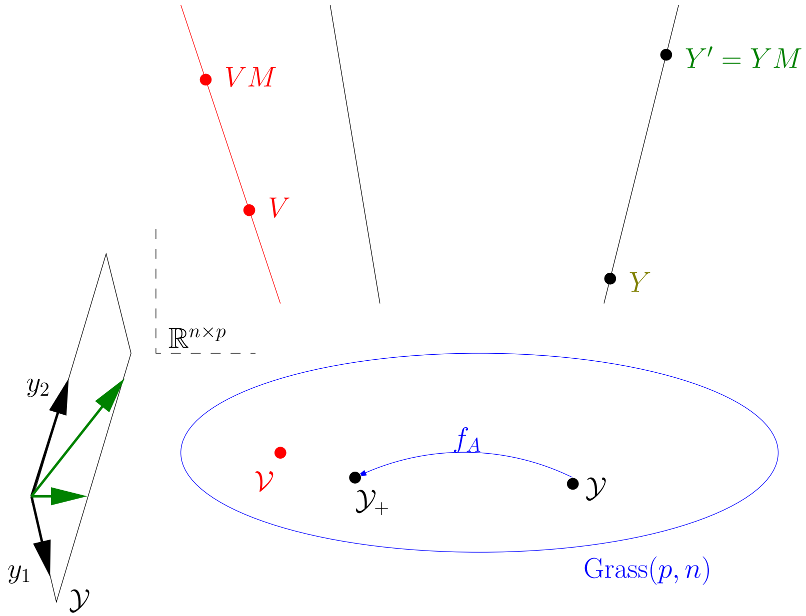
Modified Rayleigh Quotient Iteration with limited steps.

Reference: PAA, Sepulchre, Van Dooren, Mahony [ASVM03].

Refining eigenspace estimates – Main Results

- Newton methods:
  - Practical formulation of the Riemannian Newton method on the Grassmann manifold.
  - Newton method for refining eigenspace estimates. Quadratic convergence in general. Cubic convergence if $A = A^T$.
- Shifted inverse iterations:
  - Grassmannian generalization of the Rayleigh Quotient Iteration, using block shifts. Local cubic convergence to the eigenspaces of $A = A^T$.
  - Two-sided version for the nonsymmetric case.
- Study of the global behaviour of the iterations. Modified methods with large basins of attraction and high rate of convergence.

Refining eigenspace estimates – Conclusion



→ Geometry: iteration on the *Grassmann manifold* of p-planes in $\mathbb{R}^n$.

→ Dynamics: $\mathcal{Y}_{k+1} = f_A(\mathcal{Y}_k)$. Discrete dynamical system.

→ Numerical analysis: compute f_A efficiently.

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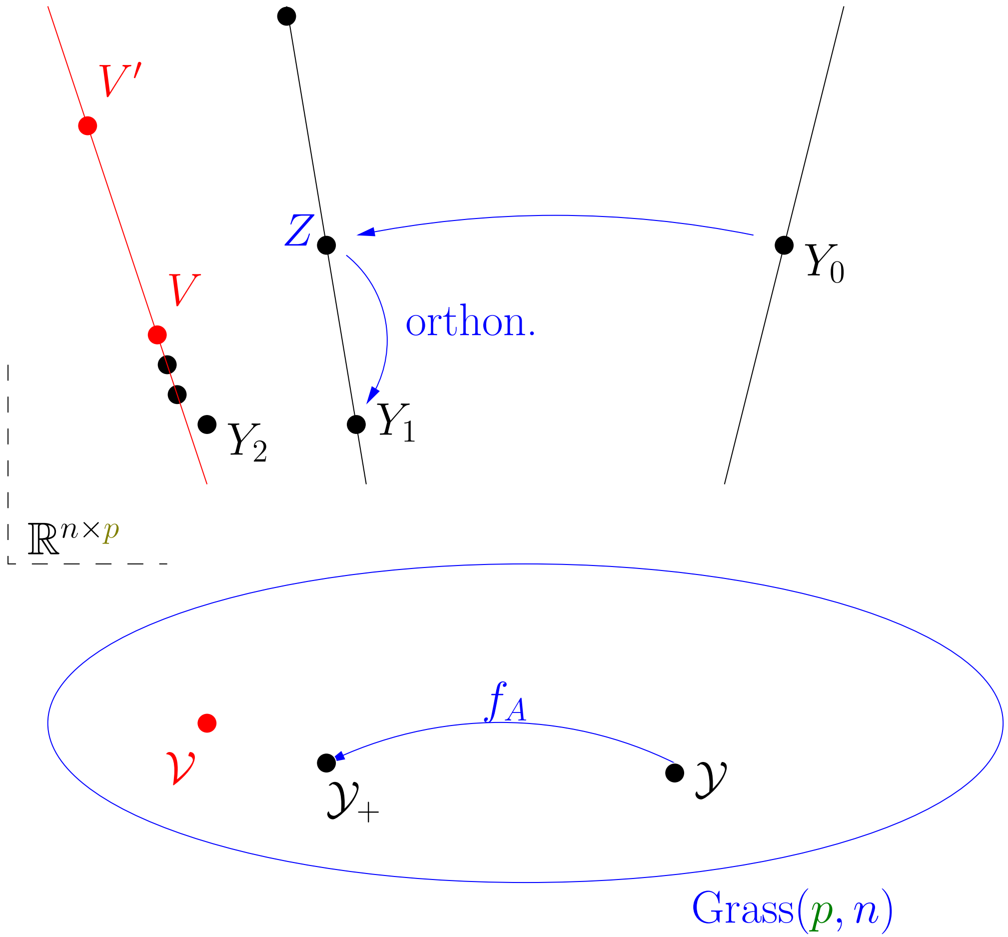
Numerical experiment:

$$AZ - ZY^T AY = Y, \; Y^T Y = I$$

$$Y_+ = \mathrm{qf}(Z).$$

```
A =
     1     0     0
     0     2     0
     0     0     3
Y =
 -1.0762e-001 -4.2770e-002
  9.9334e-001  3.6714e-002
 -4.1138e-002  9.9841e-001
Y =
 -1.3004e-003 -2.9822e-004
 -9.8317e-001 -1.8269e-001
  1.8269e-001 -9.8317e-001
Y =
 -4.4217e-011  2.3683e-009
  1.8740e-002 -9.9982e-001
 -9.9982e-001 -1.8740e-002
```

$$AZ - Z(Y^T Y)^{-1} Y^T A Y = Y$$



$$AZ - Z(Y^TY)^{-1}Y^TAY = Y$$