Sampling with constraints

Miranda Holmes-Cerfon
Courant Institute of Mathematical Sciences

Thanks to:
Jonathan Goodman
Emilio Zappa
US Dept of Energy

Zappa, H.-C., Goodman, CPAM 2018

Problem:

Sample density $\rho(x) = Z^{-1} f(x)\, \delta(q(x))\,.$

$x \in \mathbb{R}^n,\;\; f : \mathbb{R}^n \to \mathbb{R},\quad q : \mathbb{R}^n \to \mathbb{R}^m$ ("constraints".)

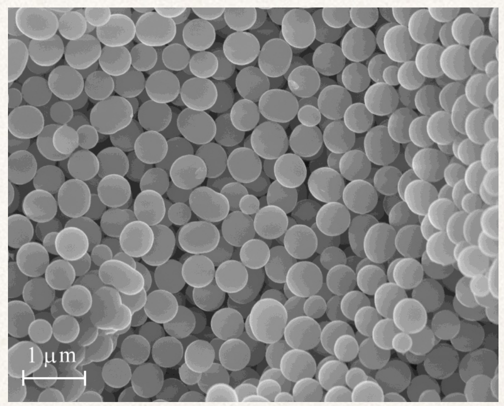
Why do this:

- Freeze out fast, vibrational degrees of freedom of strongly-bonded particles (e.g. $q(x) = |x_1 - x_2|^2 - d^2$)
- Compute Free Energy / Expectations at certain levels of a reaction coordinate
- Bayesian sampling — constraints on parameters (e.g. $p_1+p_2+p_3=1$)

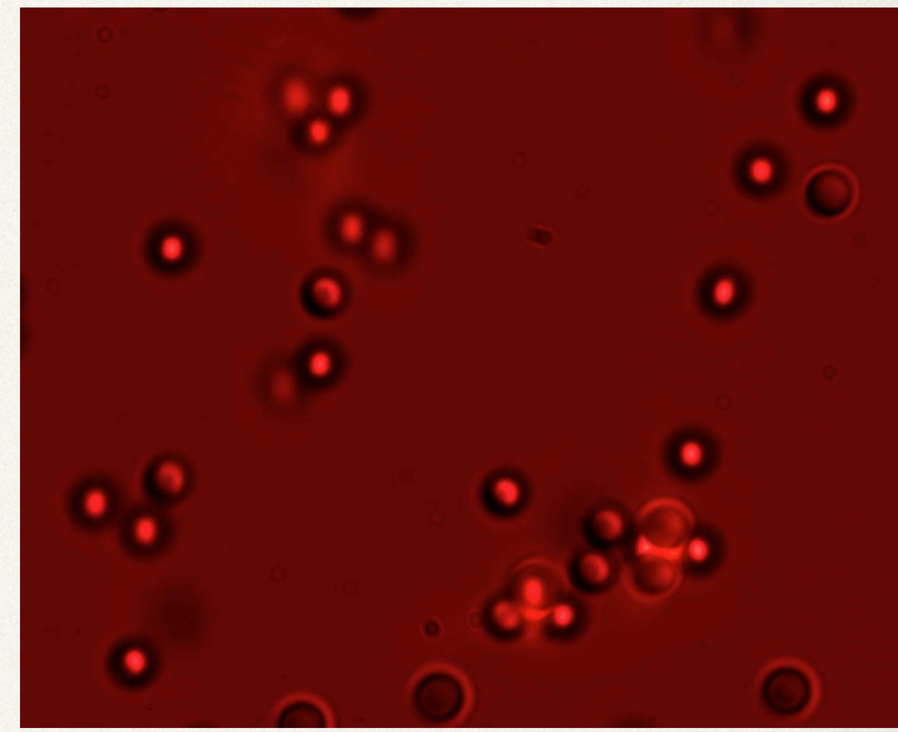
My interest = Colloids (colloidal particles)

- *Colloidal* particles: diameters ~ 10^{-8}-10^{-6} m. (» atoms, « scales of humans)
- Building blocks for many materials
- Potential to make new materials (∵ size ~ wavelength of light)

mayonnaise

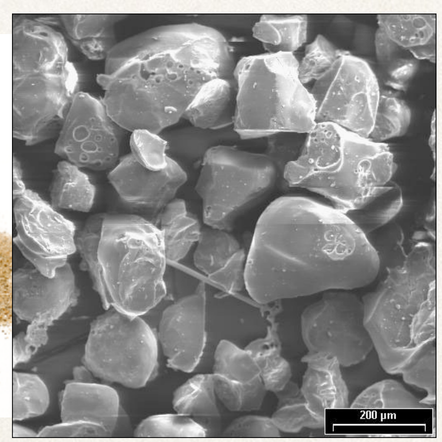


opal

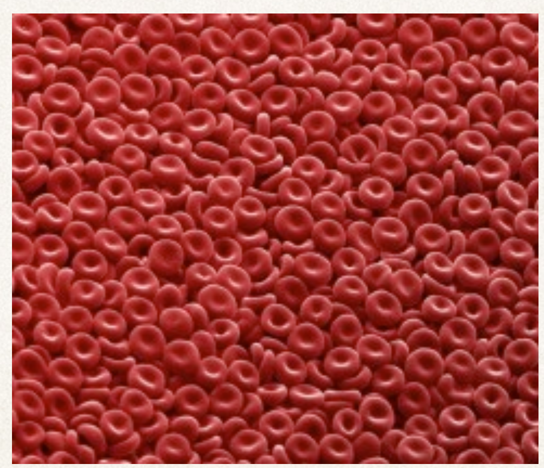


Schade, H.-C., et al. PRL (2013)

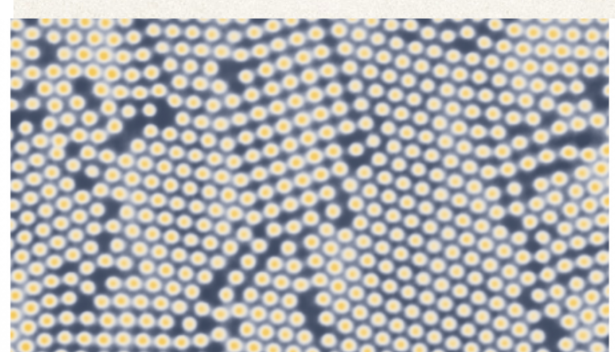
sand

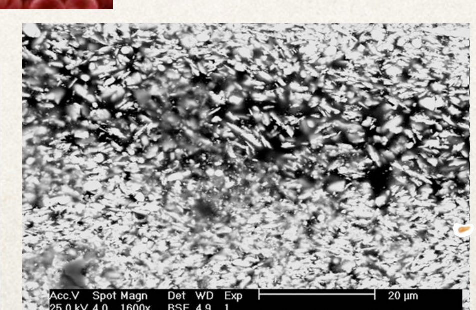


red blood cells



cornstarch





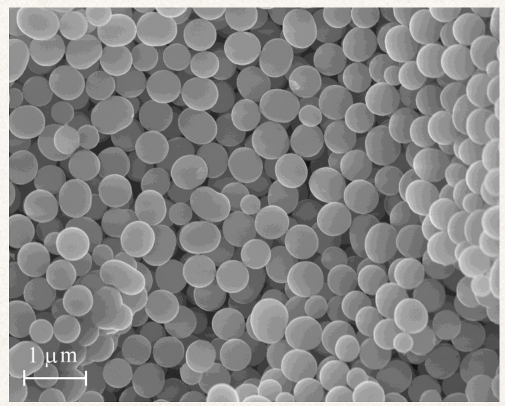
paint

ketchup

My interest = Colloids (colloidal particles)

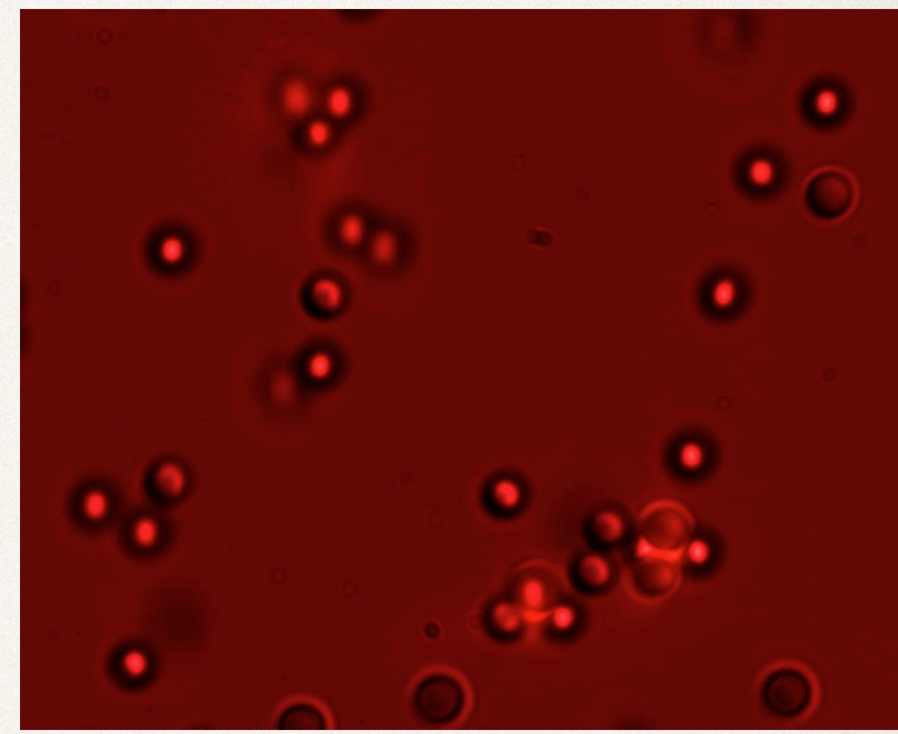
- *Colloidal* particles: diameters ~ 10^{-8}-10^{-6} m. (» atoms, « scales of humans)
- Building blocks for many materials
- Potential to make new materials (∵ size ~ wavelength of light)

mayonnaise



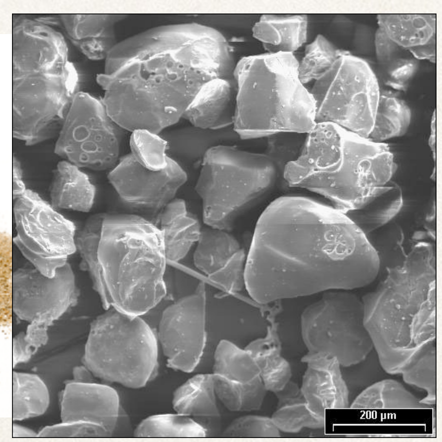
opal

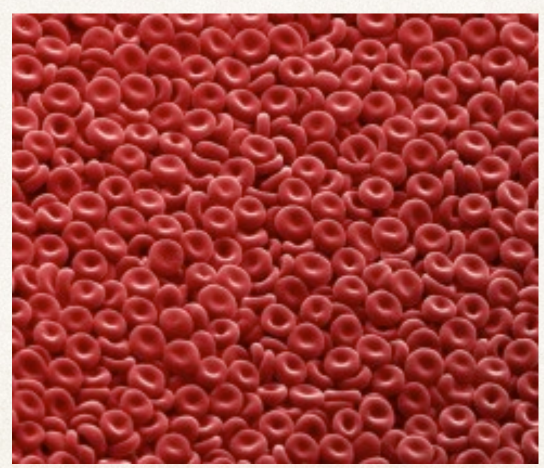
red blood cells



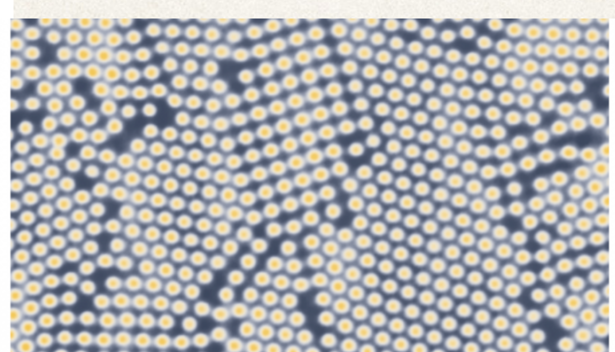
Schade, H.-C., et al. PRL (2013)

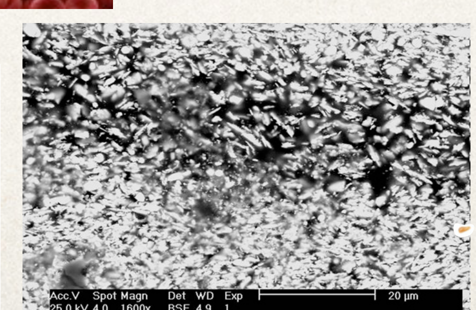
sand





cornstarch



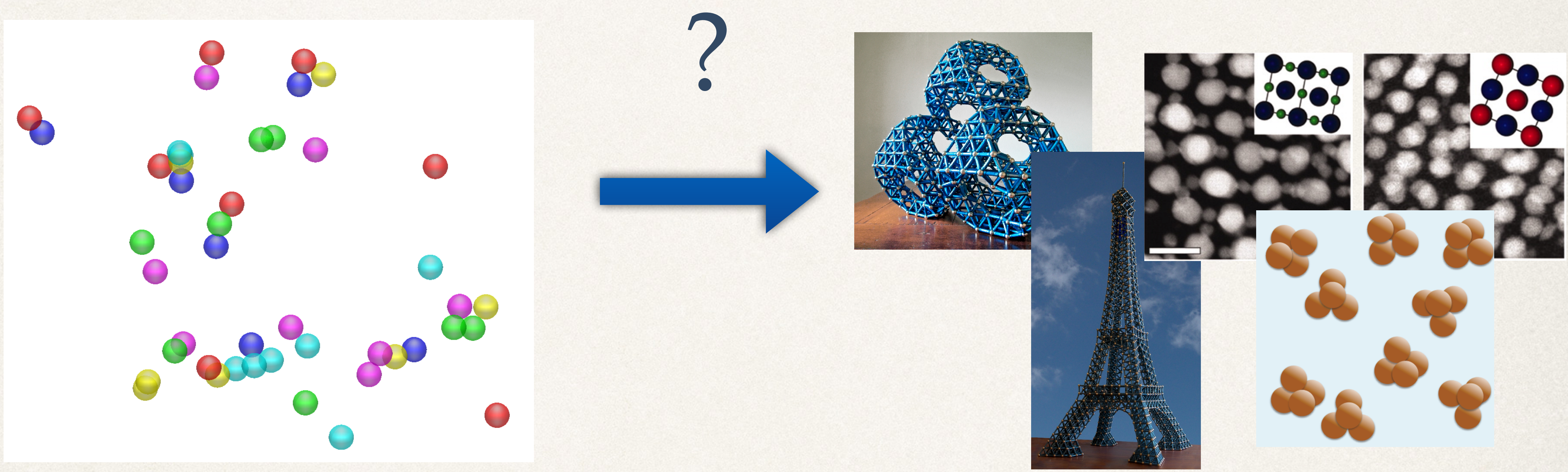


paint

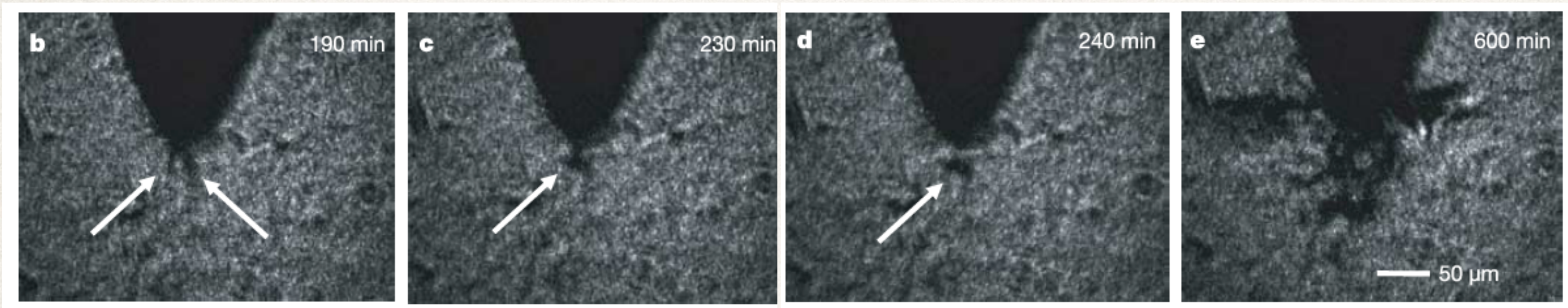
ketchup

Scientific question:

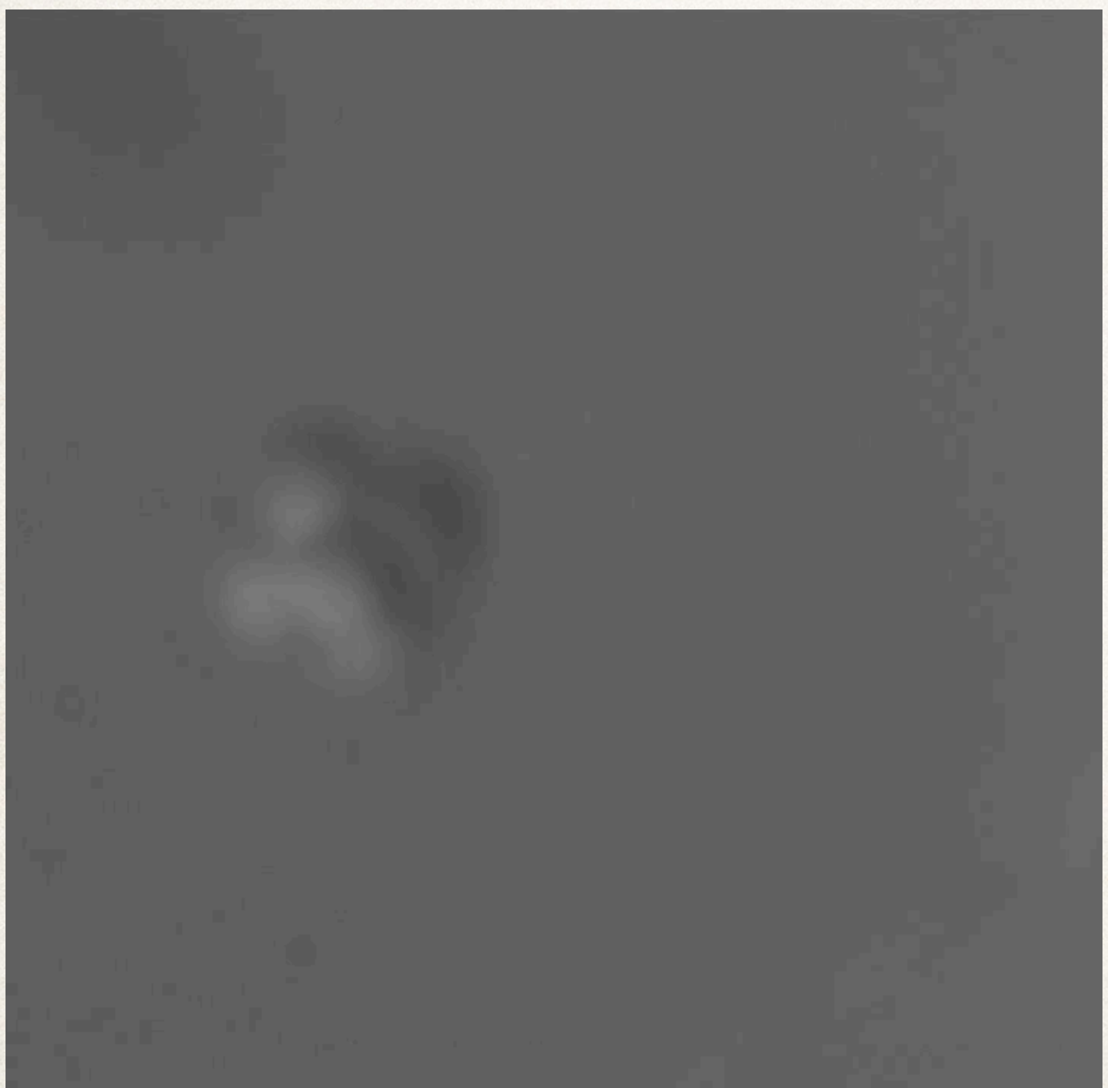
How to design colloids to self-assemble into some desired structure?

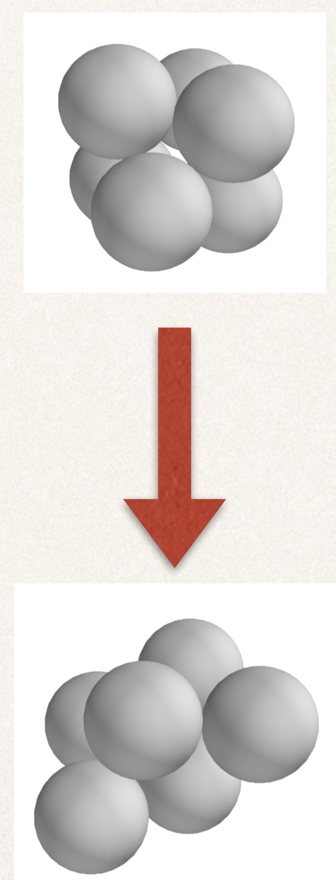


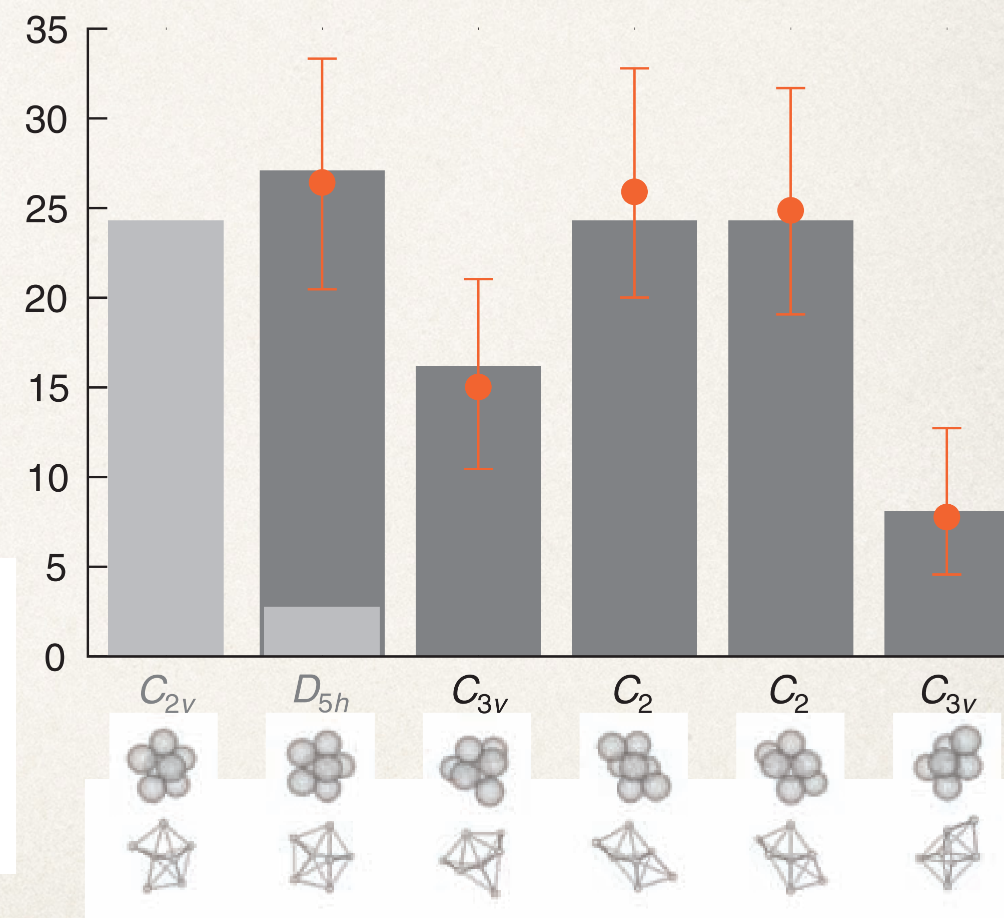
Colloids are (sometimes) easy to study experimentally



Schall et al, Nature (2006)

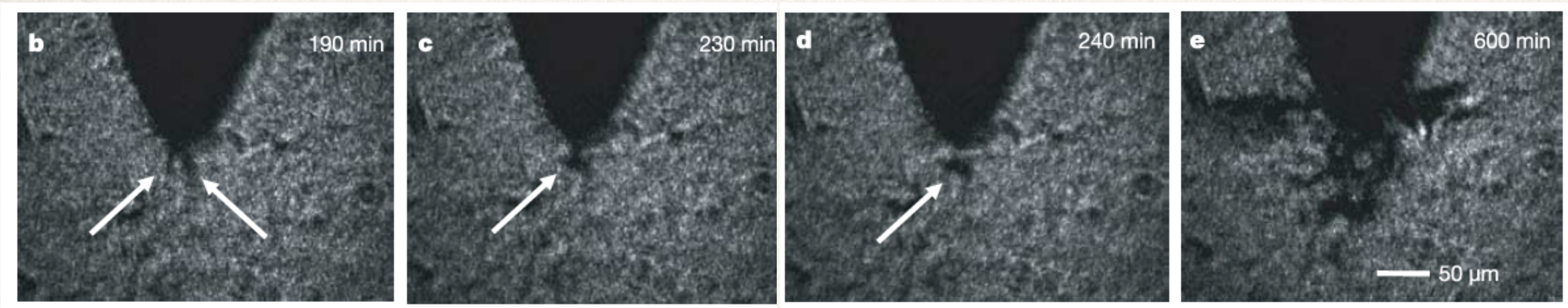




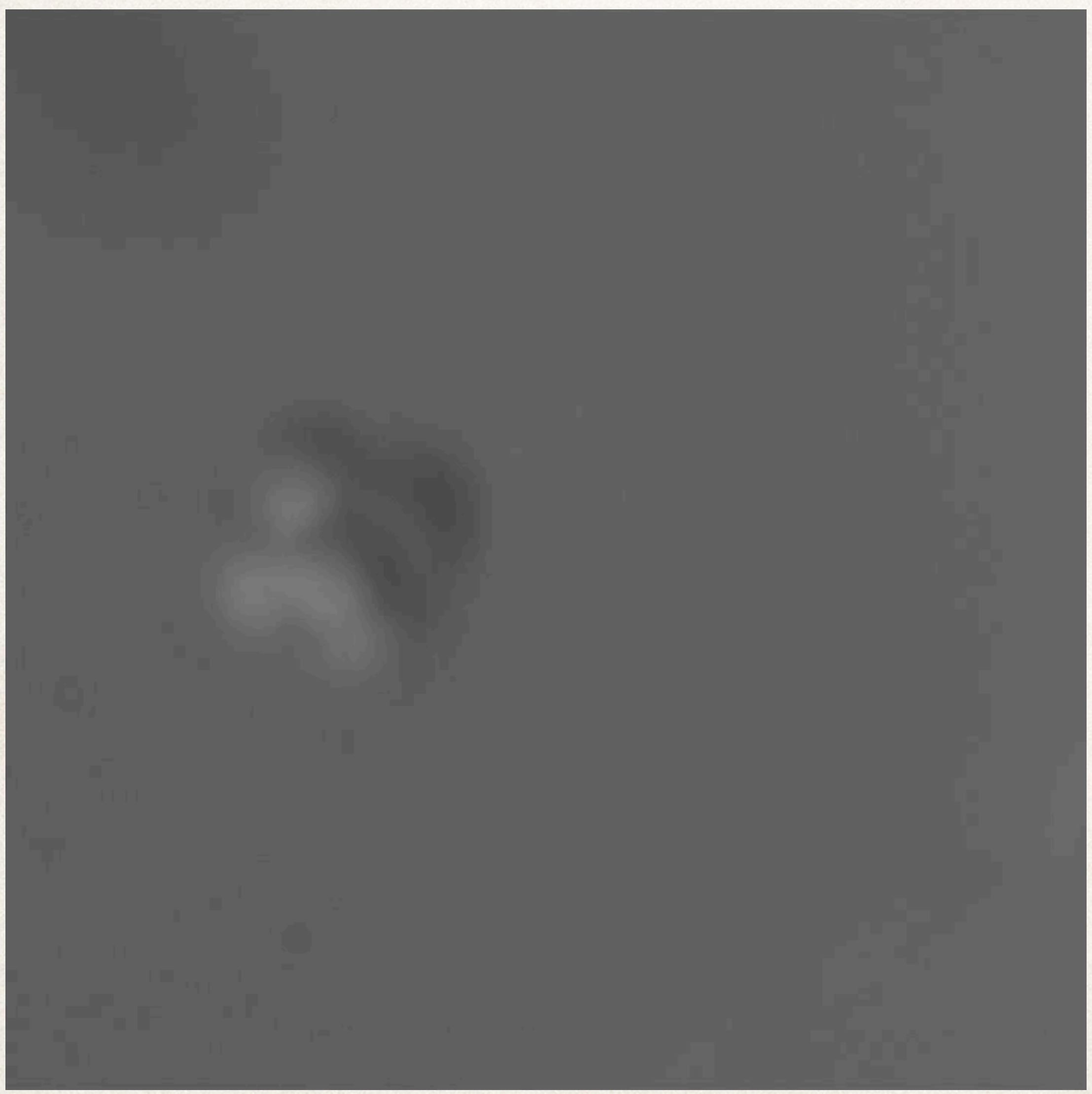


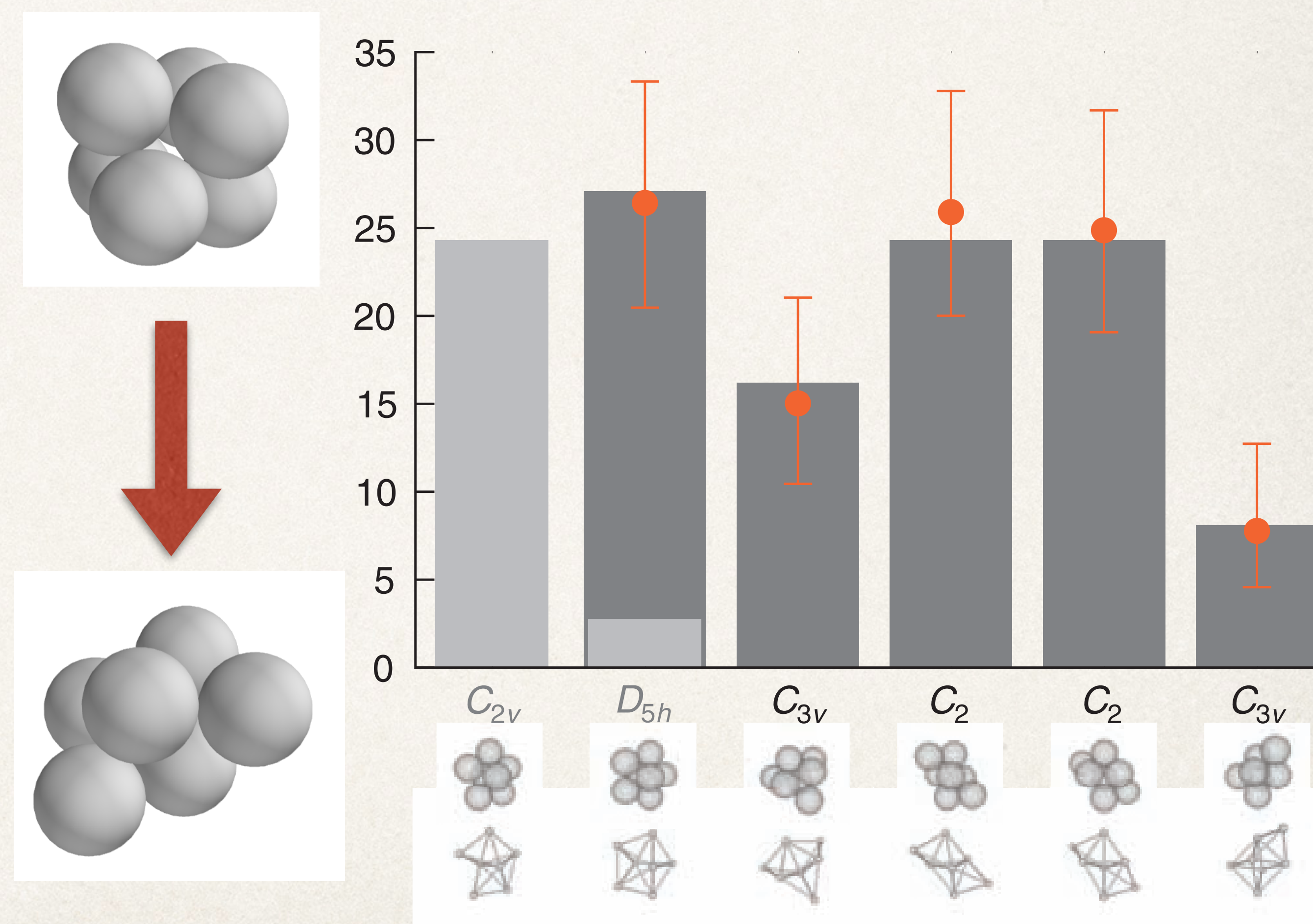
G. Meng, N. Arkus, M. P. Brenner, V. N. Manoharan, Science 327 (2010)

Colloids are (sometimes) easy to study experimentally



Schall et al, Nature (2006)

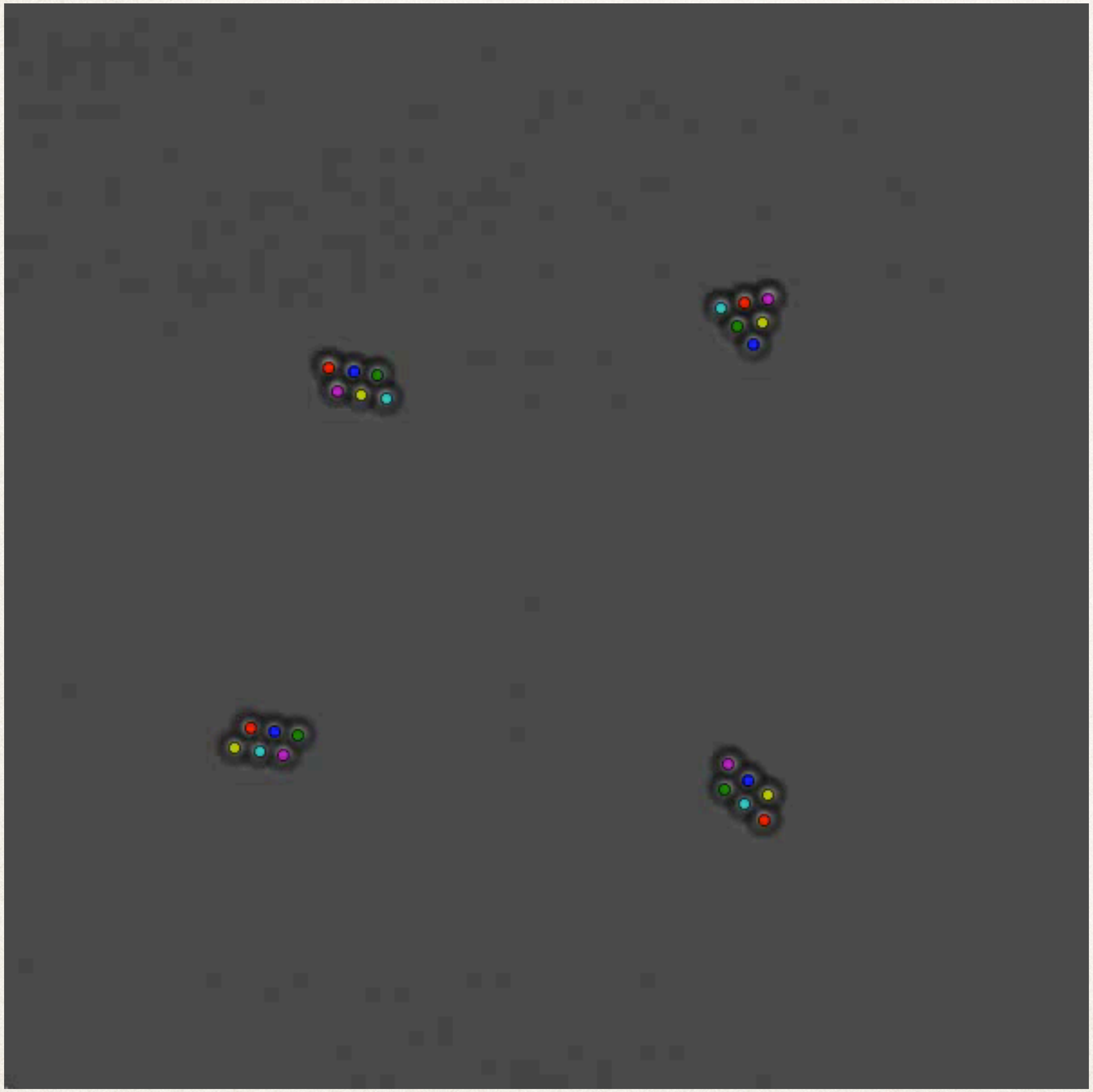


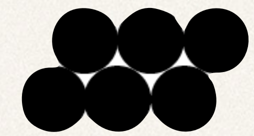
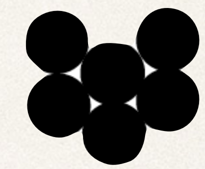
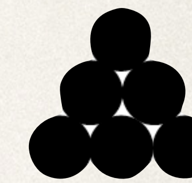
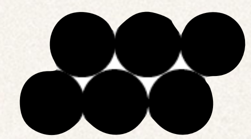
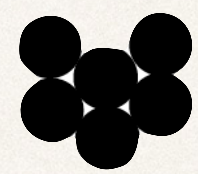
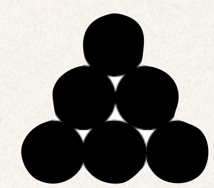


G. Meng, N. Arkus, M. P. Brenner, V. N. Manoharan, Science 327 (2010)

We can even measure dynamics with high accuracy

Rebecca Perry
(Manoharan lab)

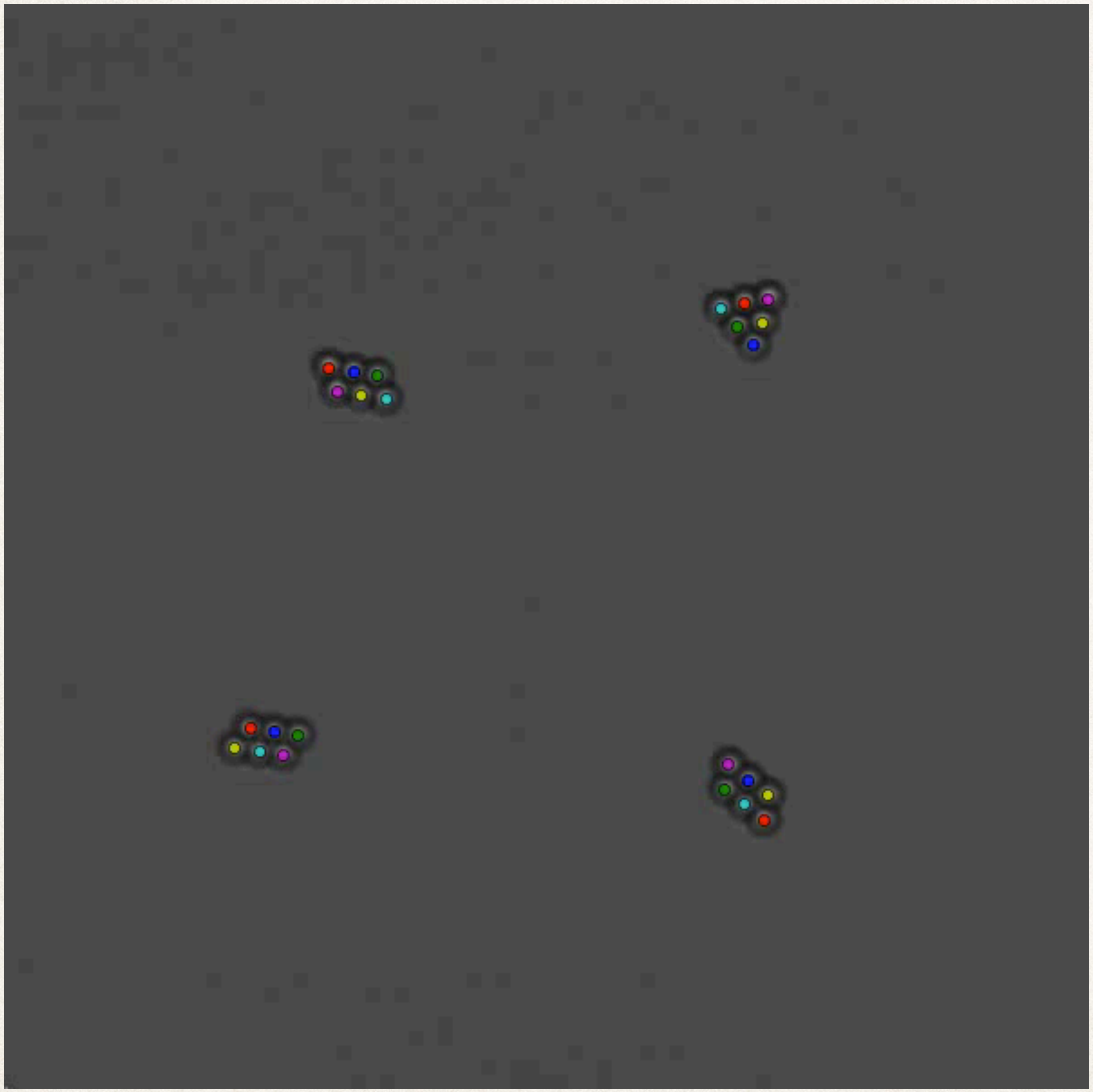


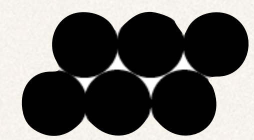
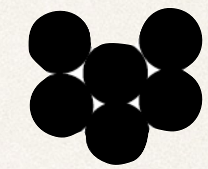
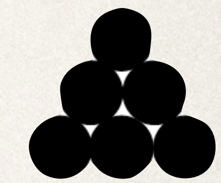
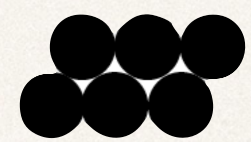
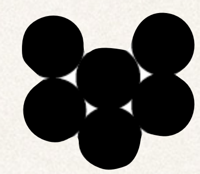
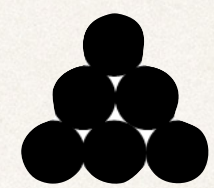
			
	112	140	64
	138	198	49
	63	55	1

R. W. Perry, H.-C., M. P. Brenner, V. N. Manoharan, PRL (2015)

We can even measure dynamics with high accuracy

Rebecca Perry
(Manoharan lab)



			
	112	140	64
	138	198	49
	63	55	1

R. W. Perry, H.-C., M. P. Brenner, V. N. Manoharan, PRL (2015)

Colloids are a lot like atoms

- Energy = pairwise interactions

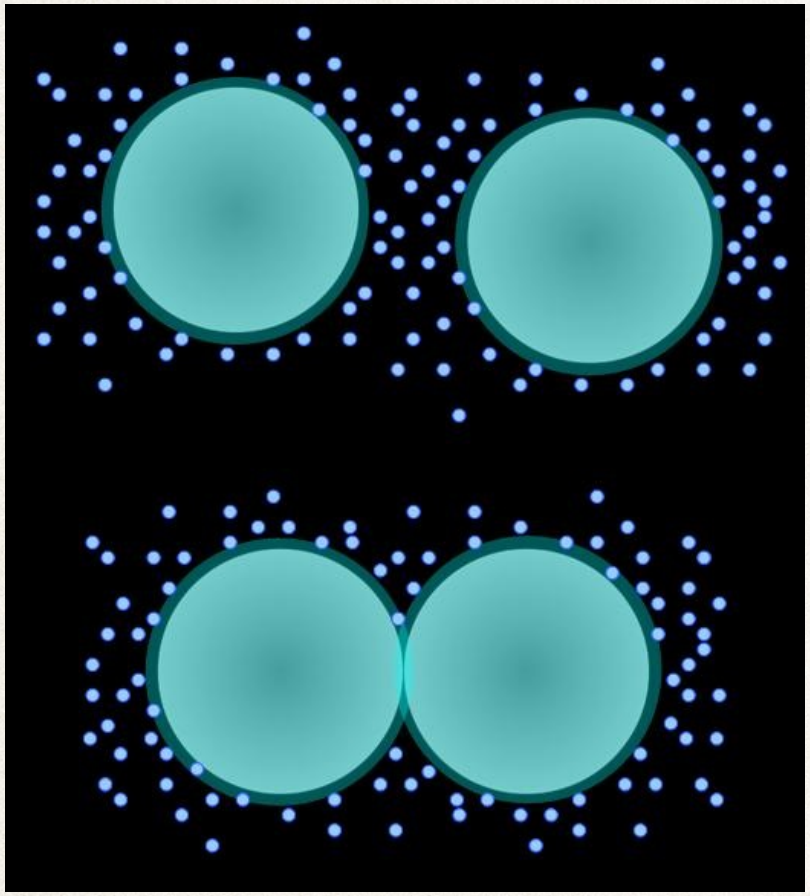
$$\pi(x) \propto e^{-\beta V(x)}, \qquad V(x) = \sum_{i<j} U(|x_i - x_j|)$$

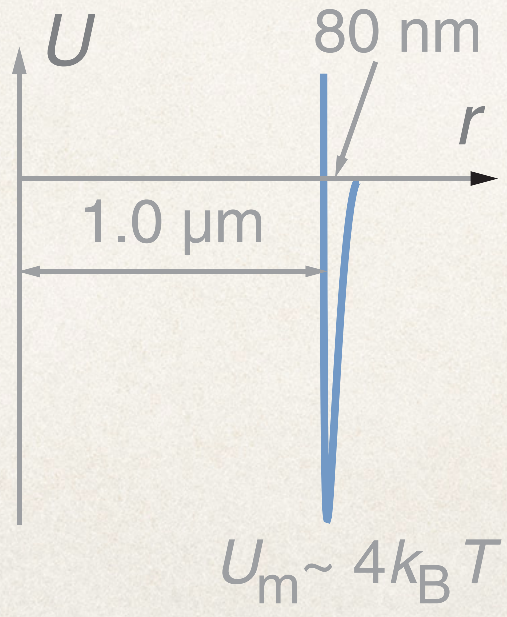
- Dynamics = overdamped Langevin

$$dX_t = \frac{-\nabla V(x)}{\gamma} dt + \sqrt{2k_B T \gamma^{-1}}\, dW_t$$

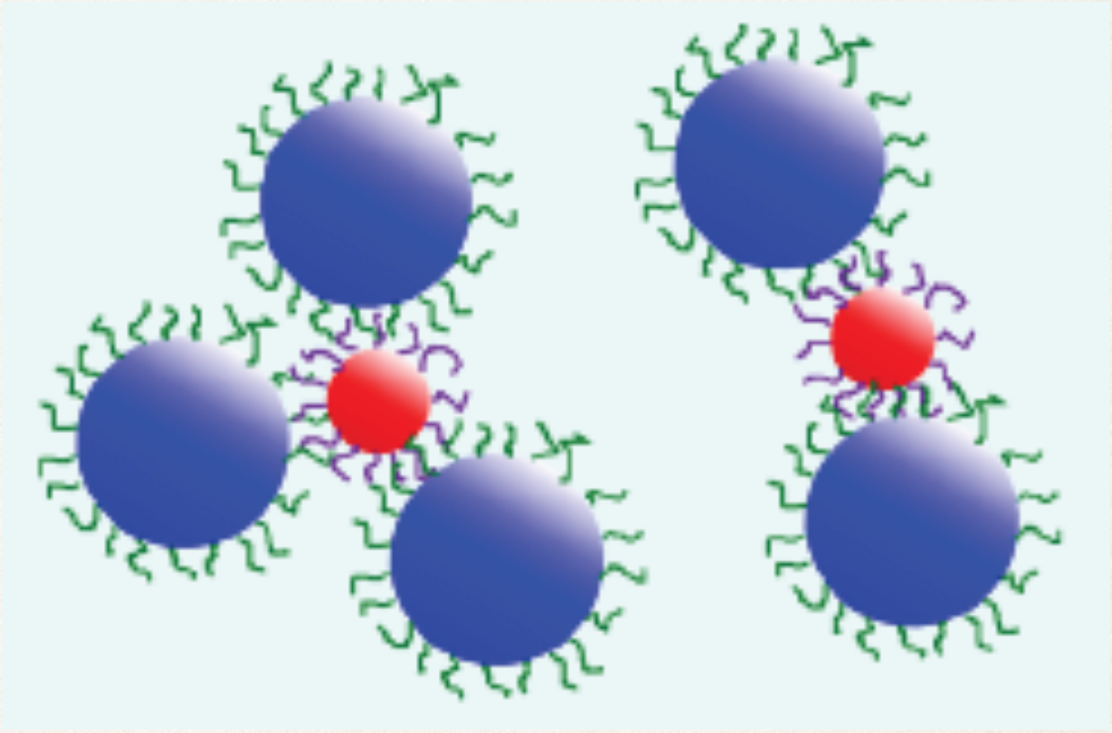
Colloids have short-ranged attractive interactions (unlike atoms)

Depletion





DNA-mediated interactions



N. Seeman, 1982

⋮

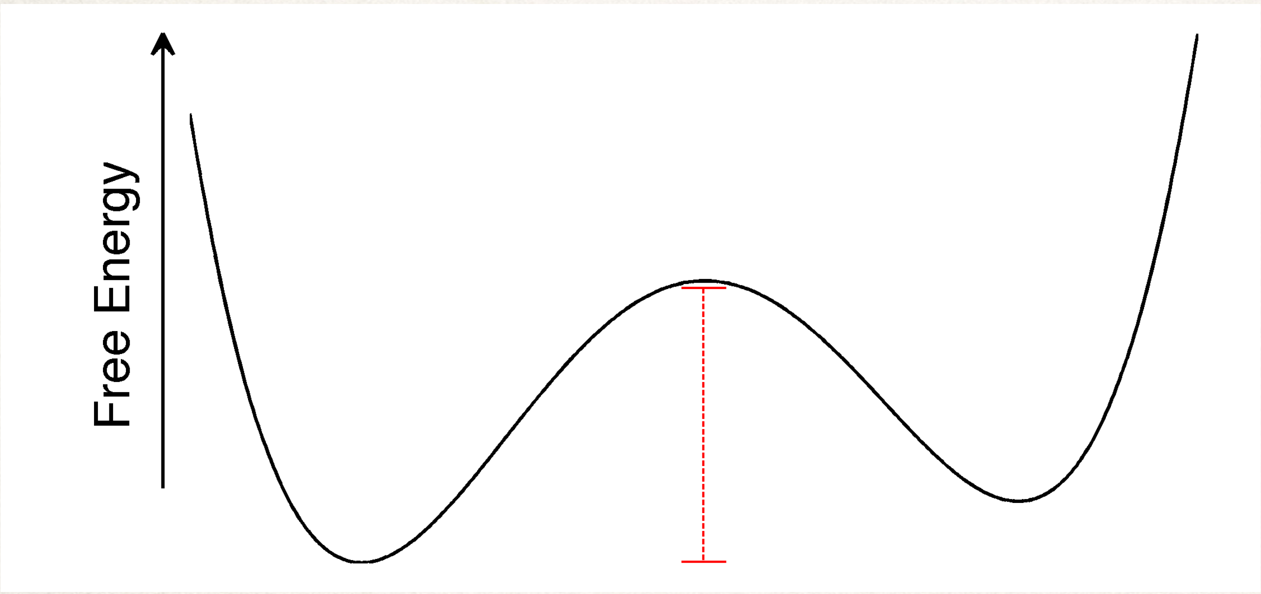
Rothemund (2006)

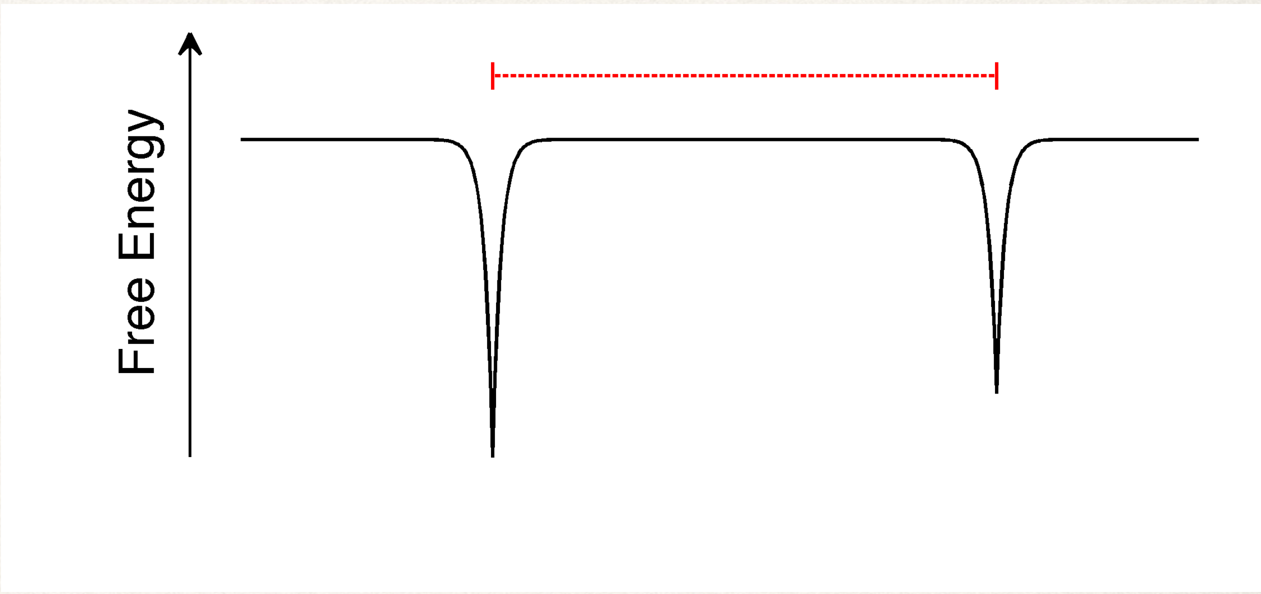
⋮

Wang et al, Nat. Comm, (2015)

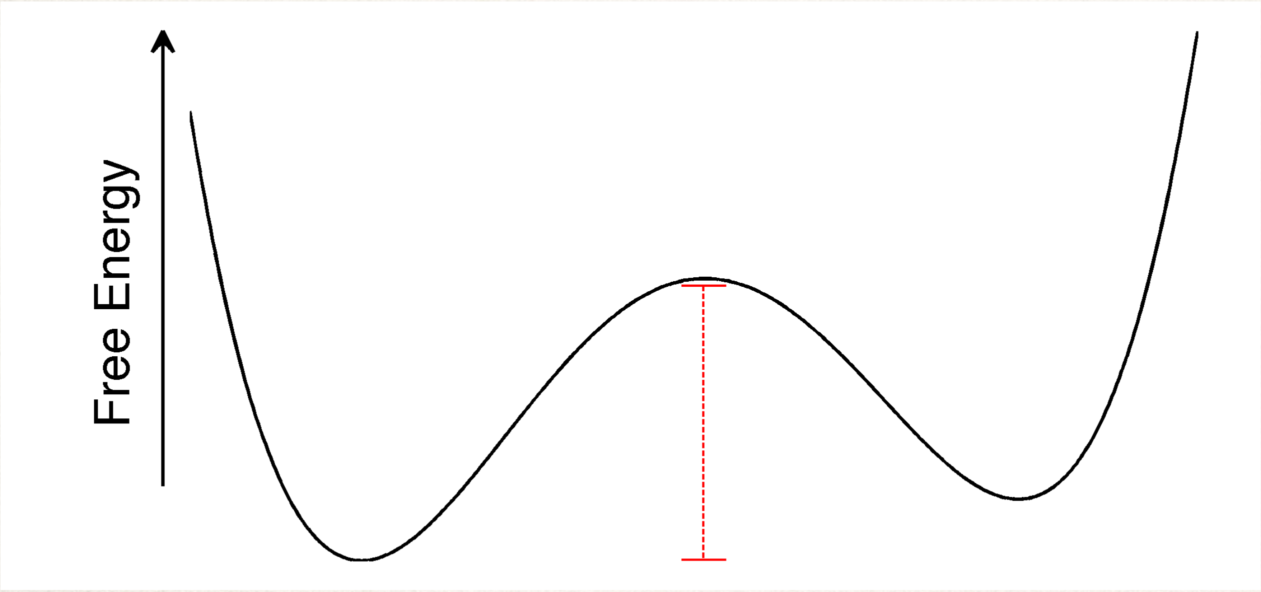
Common feature = **short-ranged** (c.f. diameter of particles)

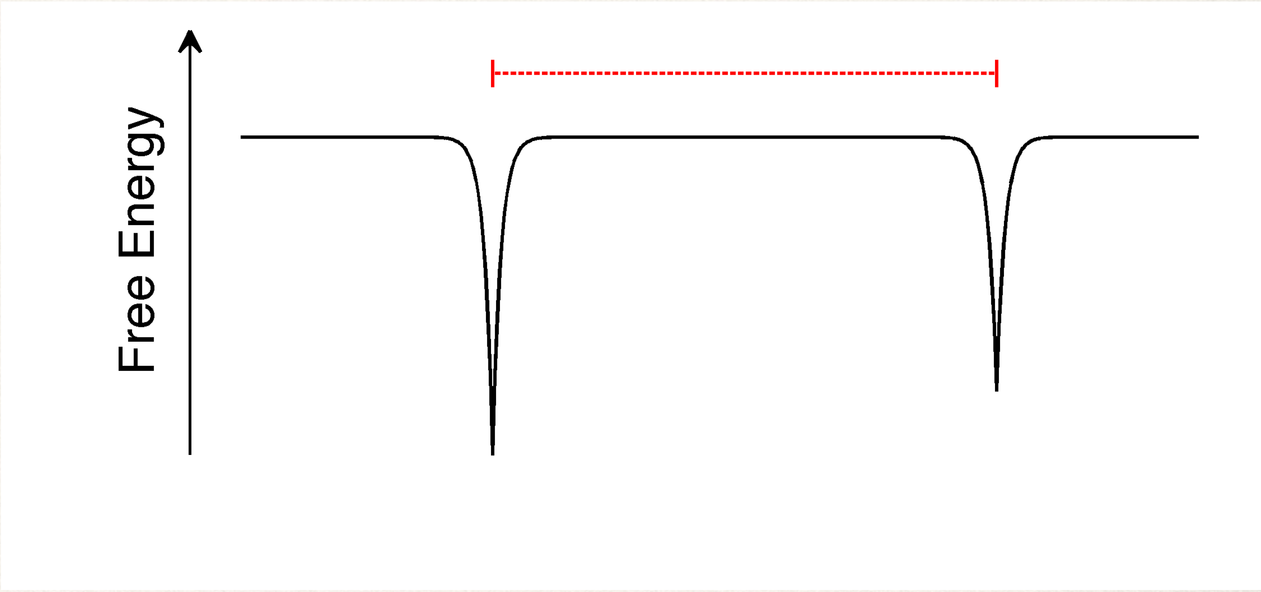
Challenges of very short-ranged interactions

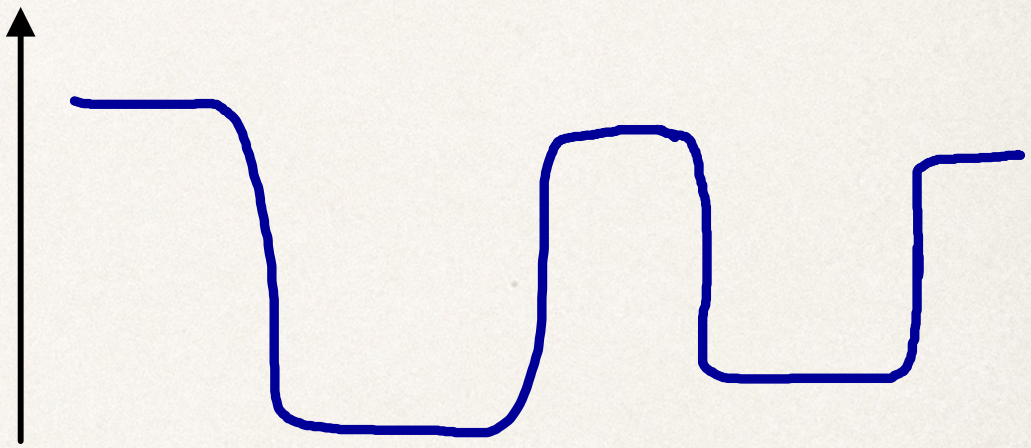




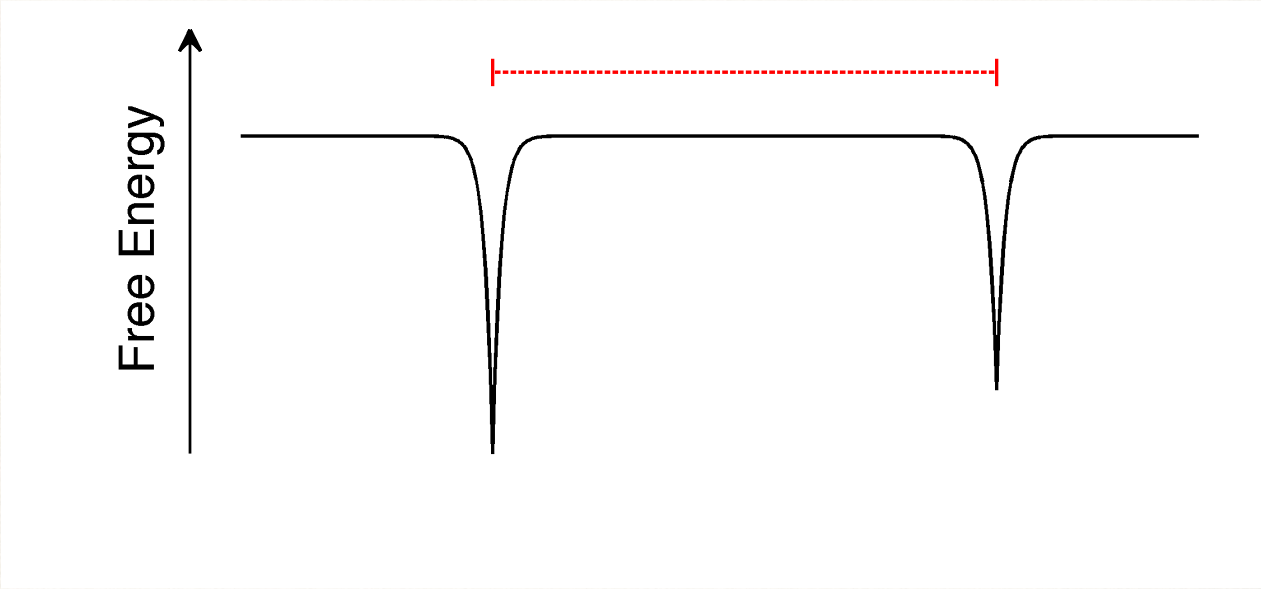
Challenges of very short-ranged interactions

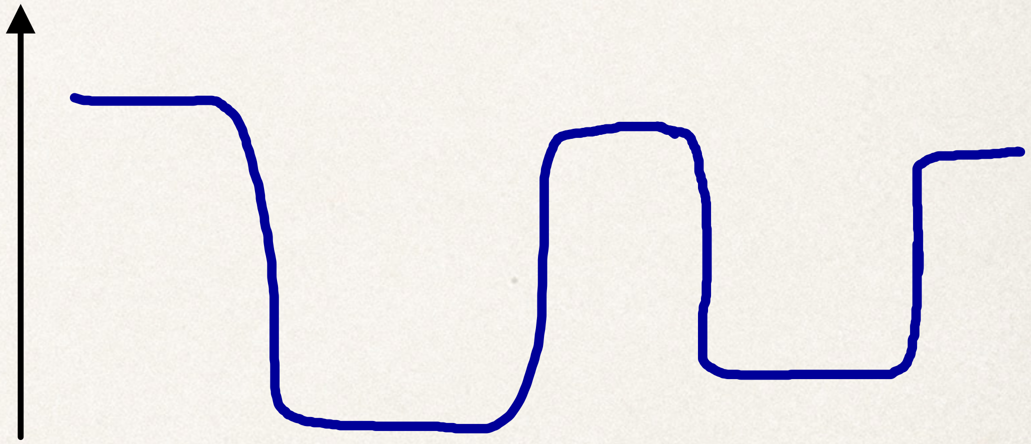




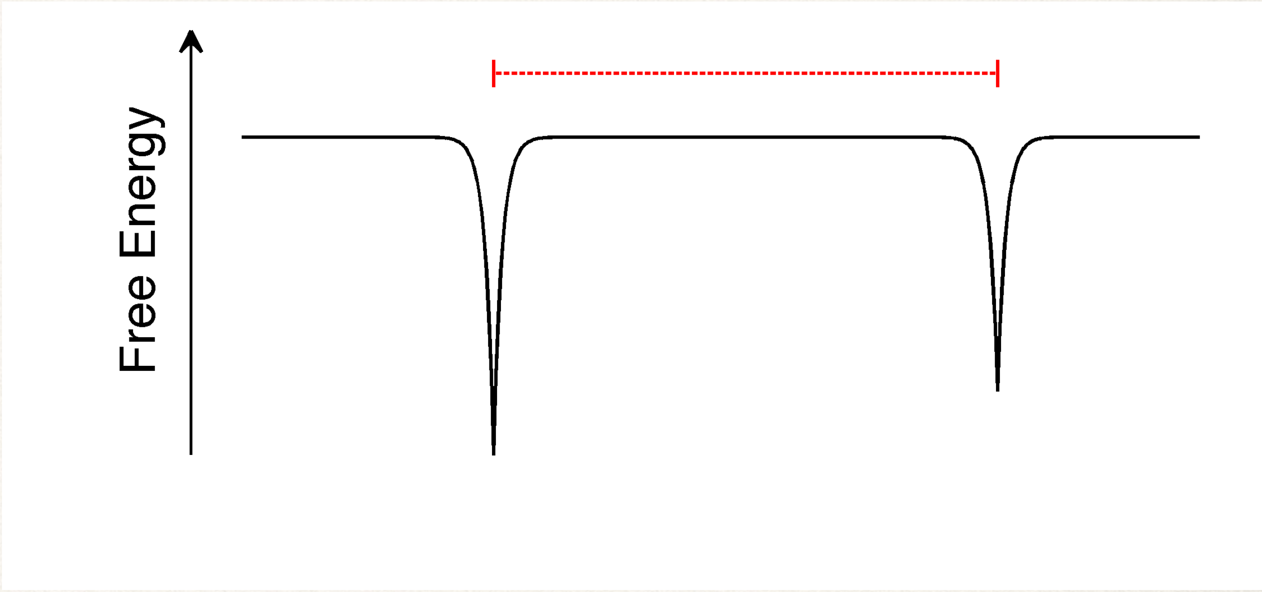


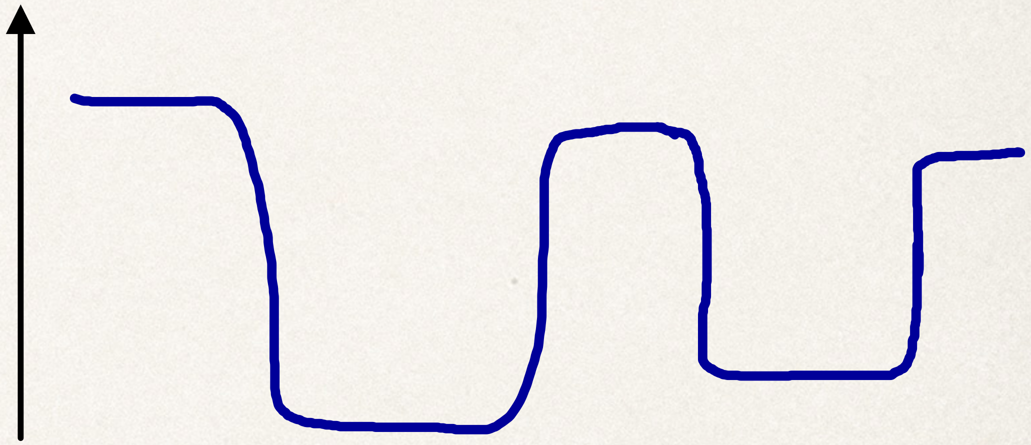
Challenges of very short-ranged interactions





Challenges of very short-ranged interactions



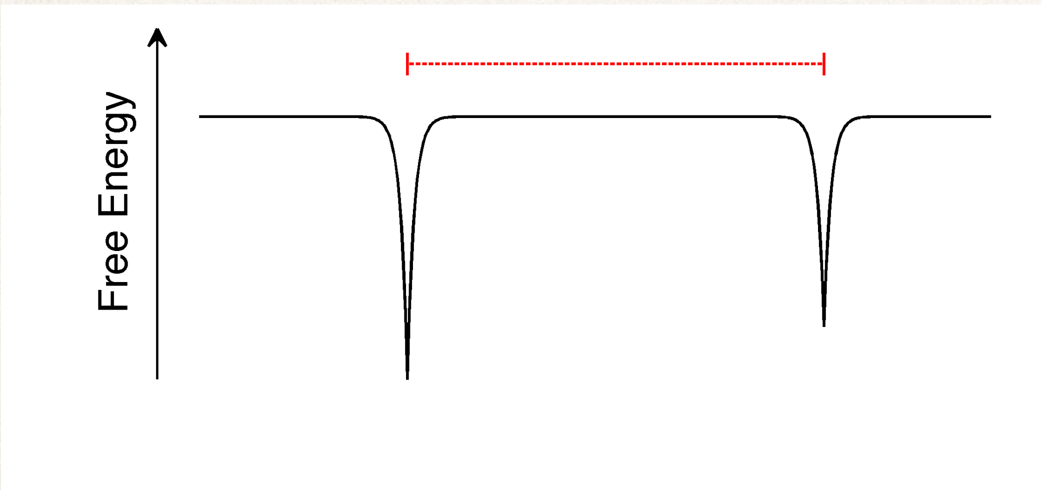


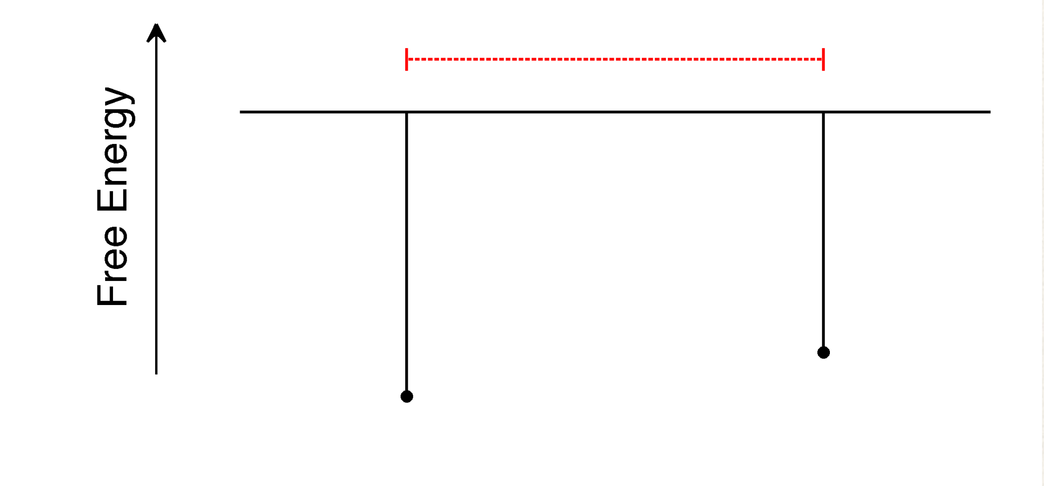
Challenges:

- **Numerical** — need a very small time step to simulate
- **Conceptual** — theories based on landscape smoothness (local minima, saddle points, etc) don't work as well

Mitigating the challenge

Shrink bonds to zero-range —> they become constraints $\delta(q)$





Need tools to:

- Sample particles with distance (or other) constraints (*this talk*)
  (to calculate volumes)
- Add & drop constraints via MCMC (*ask me later*) or in a way that is consistent with their dynamics (*work in progress with Nawaf Bou-Rabee*)
- Incorporate hydrodynamics (*e.g. Aleks Donev*) & DNA-induced dynamics
- Solve inverse problems involving their interactions (*??*)

Setup for sampling $\rho(x) = Z^{-1}\delta(q(x))$

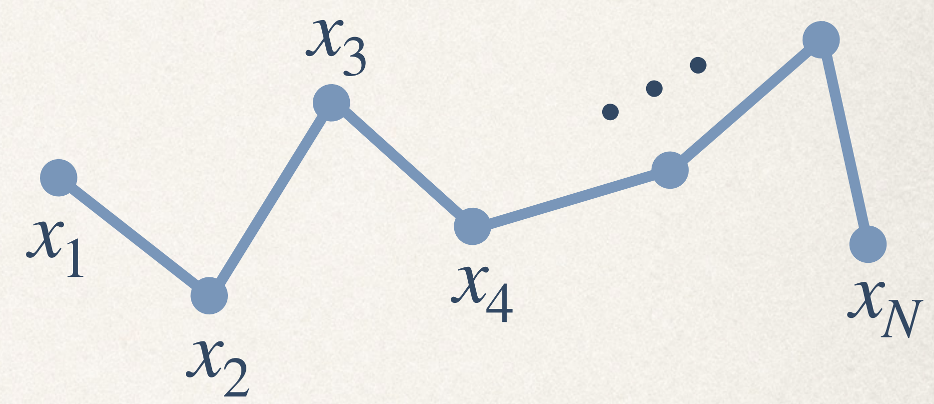
$q(x) = (q_1(x), \ldots, q_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$

Strategy: sample measure on constraint manifold

$$M = \{x \in \mathbb{R}^n : q_1(x) = 0, q_2(x) = 0, \ldots, q_m(x) = 0\}$$

e.g.

$$q_1(x) = |x_1 - x_2|^2 - d_{12}^2$$
$$q_2(x) = |x_2 - x_3|^2 - d_{23}^2$$
$$\vdots \qquad \vdots$$
$$q_{N-1}(x) = |x_{N-1} - x_N|^2 - d_{N-1N}^2$$



Setup for sampling $\rho(x) = Z^{-1}\delta(q(x))$

$q(x) = (q_1(x), \ldots, q_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$

Strategy: sample measure on constraint manifold

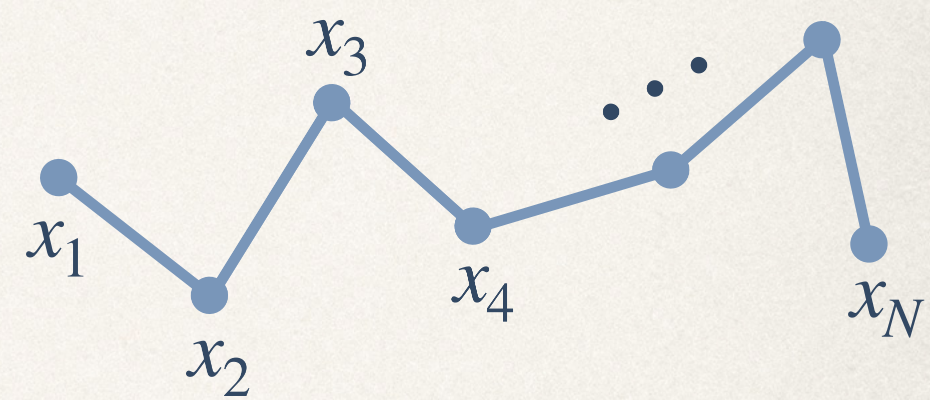
$$M = \{x \in \mathbb{R}^n : q_1(x) = 0, q_2(x) = 0, \ldots, q_m(x) = 0\}$$

Assume

$\{\nabla q_1(x), \ldots, \nabla q_m(x)\}$ linearly independent $\forall x \in M$.

e.g.

$$q_1(x) = |x_1 - x_2|^2 - d_{12}^2$$
$$q_2(x) = |x_2 - x_3|^2 - d_{23}^2$$
$$\vdots \qquad\qquad \vdots$$
$$q_{N-1}(x) = |x_{N-1} - x_N|^2 - d_{N-1N}^2$$



Setup for sampling $\rho(x) = Z^{-1}\delta(q(x))$

$q(x) = (q_1(x), \dots, q_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$

Strategy: sample measure on constraint manifold

$$M = \{x \in \mathbb{R}^n : q_1(x) = 0, q_2(x) = 0, \dots, q_m(x) = 0\}$$

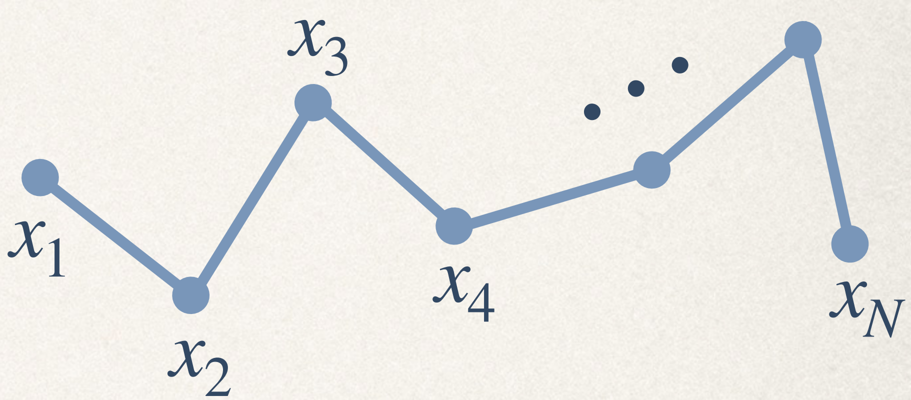
Assume

$\{\nabla q_1(x), \dots, \nabla q_m(x)\}$ linearly independent $\forall x \in M$.

- implies M is a manifold (dimension d=n-m)

e.g.

$$q_1(x) = |x_1 - x_2|^2 - d_{12}^2$$
$$q_2(x) = |x_2 - x_3|^2 - d_{23}^2$$
$$\vdots \qquad \vdots$$
$$q_{N-1}(x) = |x_{N-1} - x_N|^2 - d_{N-1N}^2$$



Setup for sampling $\rho(x) = Z^{-1}\delta(q(x))$

$q(x) = (q_1(x), \ldots, q_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$

Strategy: sample measure on constraint manifold

$$M = \{x \in \mathbb{R}^n : q_1(x) = 0, q_2(x) = 0, \ldots, q_m(x) = 0\}$$

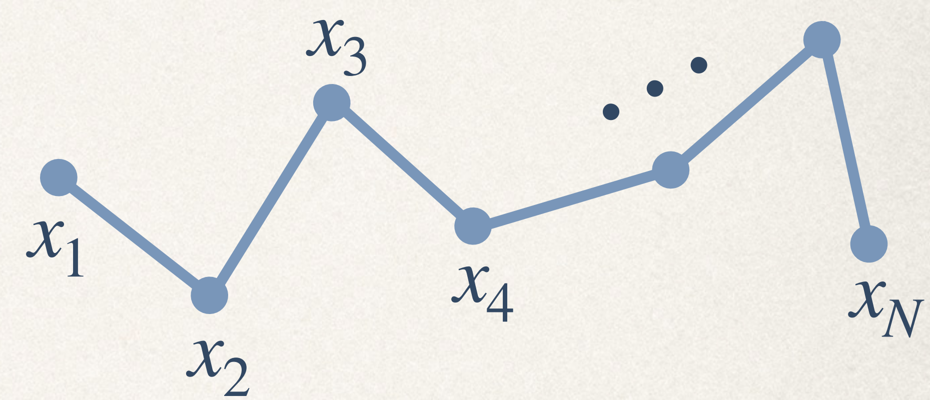
Assume

$\{\nabla q_1(x), \ldots, \nabla q_m(x)\}$ linearly independent $\forall x \in M$.

- implies M is a manifold (dimension d=n-m)
- doesn't always have to hold!
  (and even when it does, won't necessarily hold ∀x)

e.g.

$$q_1(x) = |x_1 - x_2|^2 - d_{12}^2$$
$$q_2(x) = |x_2 - x_3|^2 - d_{23}^2$$
$$\vdots \qquad\qquad \vdots$$
$$q_{N-1}(x) = |x_{N-1} - x_N|^2 - d_{N-1N}^2$$



Setup for sampling $\rho(x) = Z^{-1}\delta(q(x))$

$q(x) = (q_1(x), \ldots, q_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$

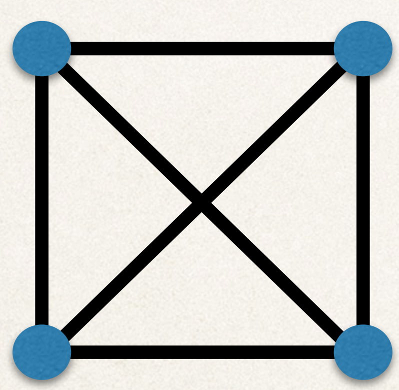
Strategy: sample measure on constraint manifold

$$M = \{x \in \mathbb{R}^n : q_1(x) = 0, q_2(x) = 0, \ldots, q_m(x) = 0\}$$

Assume

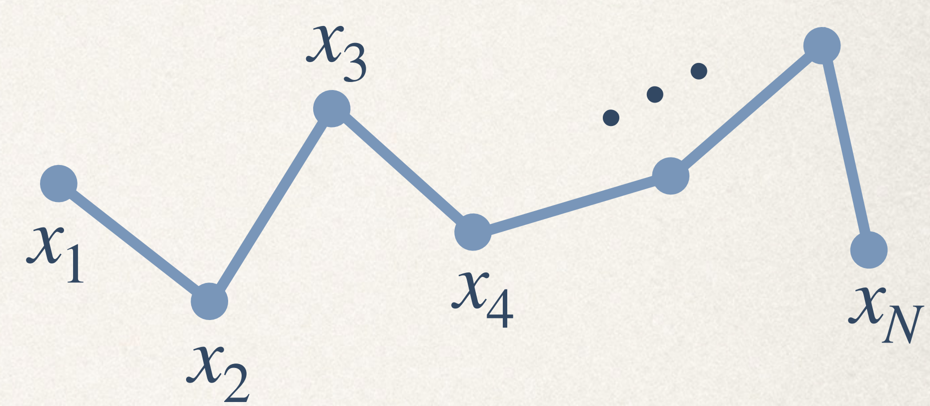
$\{\nabla q_1(x), \ldots, \nabla q_m(x)\}$ linearly independent $\forall x \in M$.

- implies M is a manifold (dimension d=n-m)
- doesn't always have to hold!
  (and even when it does, won't necessarily hold ∀x)



e.g.

$$q_1(x) = |x_1 - x_2|^2 - d_{12}^2$$
$$q_2(x) = |x_2 - x_3|^2 - d_{23}^2$$
$$\vdots \qquad \vdots$$
$$q_{N-1}(x) = |x_{N-1} - x_N|^2 - d_{N-1N}^2$$



Setup for sampling $\rho(x) = Z^{-1}\delta(q(x))$

$q(x) = (q_1(x), \ldots, q_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$

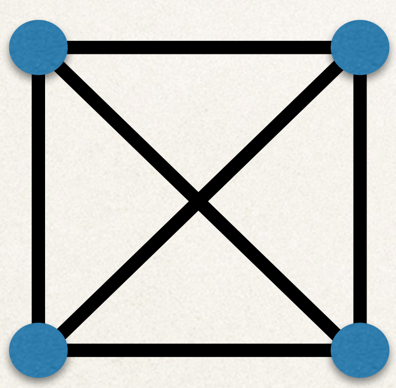
Strategy: sample measure on constraint manifold

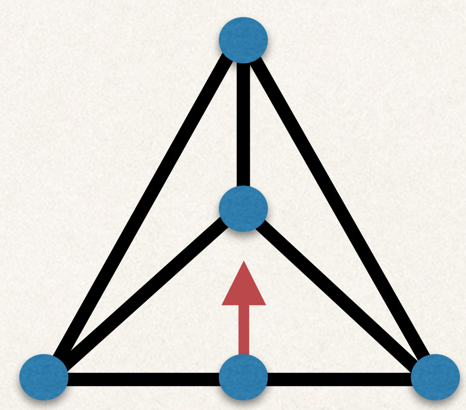
$$M = \{x \in \mathbb{R}^n : q_1(x) = 0, q_2(x) = 0, \ldots, q_m(x) = 0\}$$

Assume

$\{\nabla q_1(x), \ldots, \nabla q_m(x)\}$ linearly independent $\forall x \in M$.

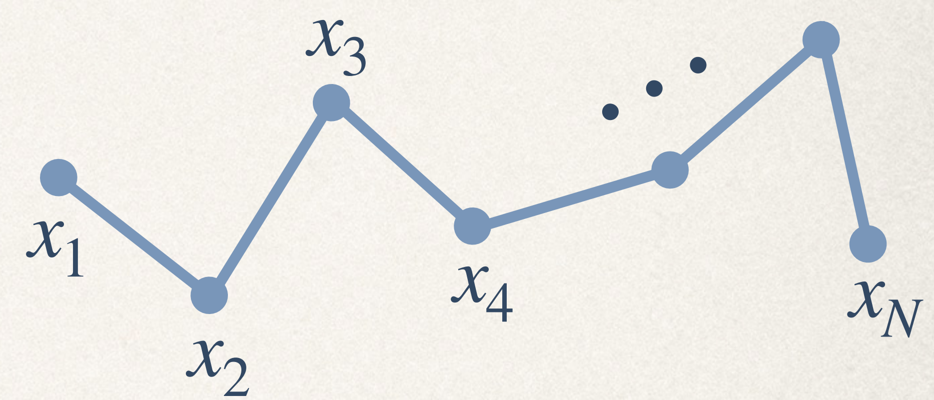
- implies M is a manifold (dimension d=n-m)
- doesn't always have to hold!
  (and even when it does, won't necessarily hold ∀x)





e.g.

$$q_1(x) = |x_1 - x_2|^2 - d_{12}^2$$
$$q_2(x) = |x_2 - x_3|^2 - d_{23}^2$$
$$\vdots \qquad \vdots$$
$$q_{N-1}(x) = |x_{N-1} - x_N|^2 - d_{N-1N}^2$$



Setup for sampling $\rho(x) = Z^{-1}\delta(q(x))$

$q(x) = (q_1(x), \ldots, q_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$

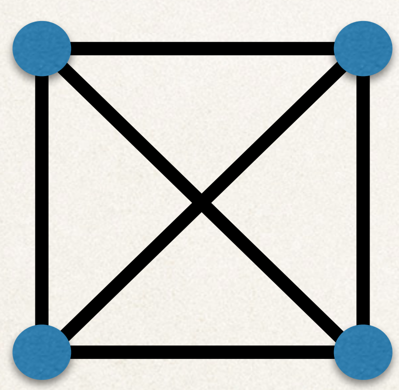
Strategy: sample measure on constraint manifold

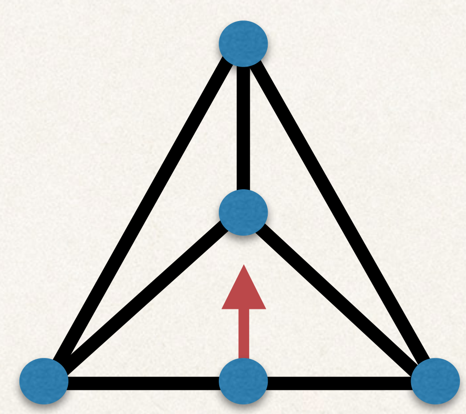
$$M = \{x \in \mathbb{R}^n : q_1(x) = 0, q_2(x) = 0, \ldots, q_m(x) = 0\}$$

Assume

$\{\nabla q_1(x), \ldots, \nabla q_m(x)\}$ linearly independent $\forall x \in M$.

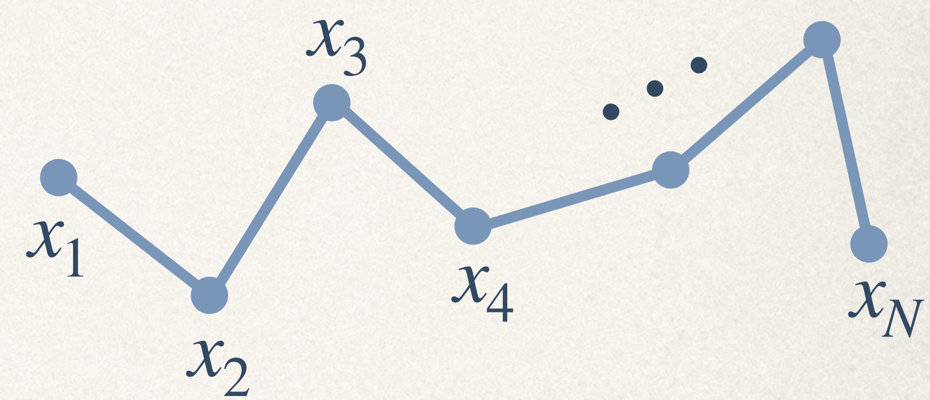
- implies M is a manifold (dimension d=n-m)
- doesn't always have to hold!
  (and even when it does, won't necessarily hold ∀x)





e.g.

$$q_1(x) = |x_1 - x_2|^2 - d_{12}^2$$
$$q_2(x) = |x_2 - x_3|^2 - d_{23}^2$$
$$\vdots \qquad\qquad \vdots$$
$$q_{N-1}(x) = |x_{N-1} - x_N|^2 - d_{N-1N}^2$$



Given $\sigma(dx)$ = natural surface measure on M (=Hausdorff measure)

Setup for sampling $\rho(x) = Z^{-1}\delta(q(x))$

$q(x) = (q_1(x), \ldots, q_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$

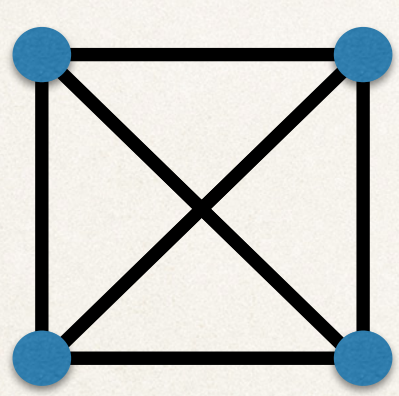
Strategy: sample measure on constraint manifold

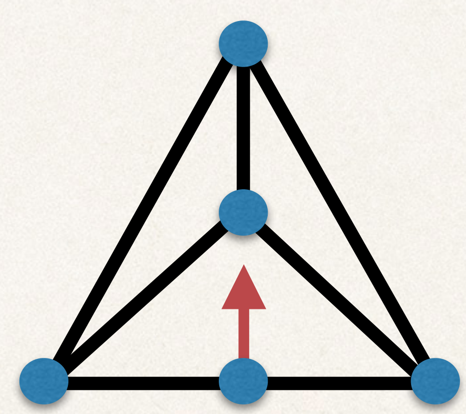
$$M = \{x \in \mathbb{R}^n : q_1(x) = 0, q_2(x) = 0, \ldots, q_m(x) = 0\}$$

Assume

$\{\nabla q_1(x), \ldots, \nabla q_m(x)\}$ linearly independent $\forall x \in M$.

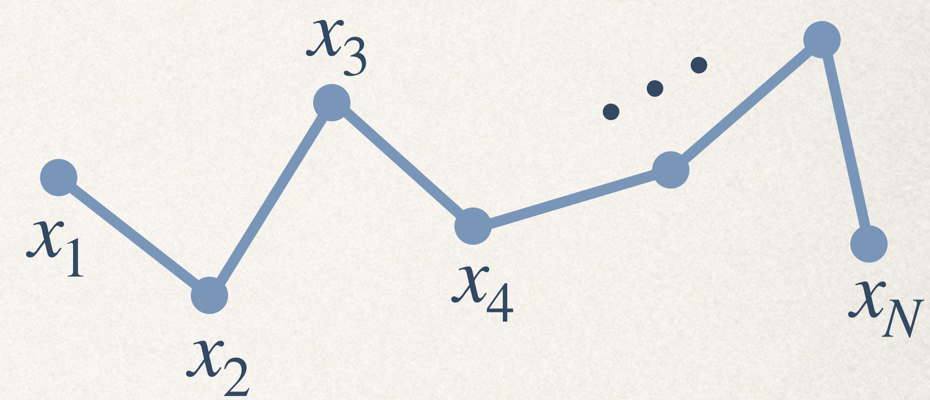
- implies M is a manifold (dimension d=n-m)
- doesn't always have to hold!
  (and even when it does, won't necessarily hold ∀x)





e.g.

$$q_1(x) = |x_1 - x_2|^2 - d_{12}^2$$
$$q_2(x) = |x_2 - x_3|^2 - d_{23}^2$$
$$\vdots \qquad \vdots$$
$$q_{N-1}(x) = |x_{N-1} - x_N|^2 - d_{N-1N}^2$$



Given $\sigma(dx)$ = natural surface measure on M (=Hausdorff measure)

Sample density $\rho(x) = f(x)\,\sigma(dx)$ s.t $f(x)\sigma(dx) = \delta(q(x))dx$

Two questions for today:

- What is f(x) so that $f(x)\sigma(dx) = \delta(q(x))dx$?
- How to sample the measure $\rho(x) = Z^{-1}f(x)\sigma(dx)$?

Then some examples!

What is f(x) so that $f(x)\sigma(dx) = \delta(q(x))dx$?

Fatten constraints by some amount ε :

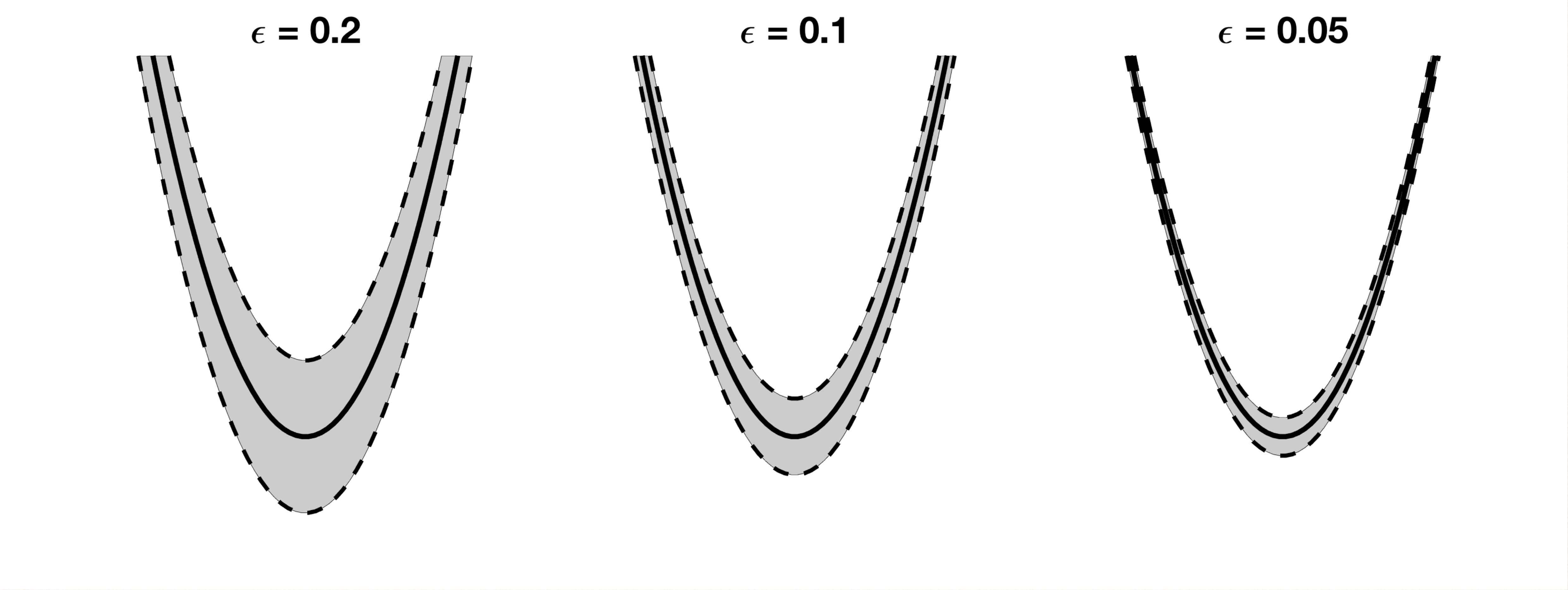
$$M^{\epsilon} = \{x \in \mathbb{R}^n : -\epsilon < q_i(x) < \epsilon, \quad i = 1,\ldots,m\}$$

Sample M^{ϵ} uniformly —> density $\rho^{\epsilon}(x)$

Then $$\delta(q(x)) = \lim_{\epsilon \to 0} \rho^{\epsilon}(x)\,.$$

Example

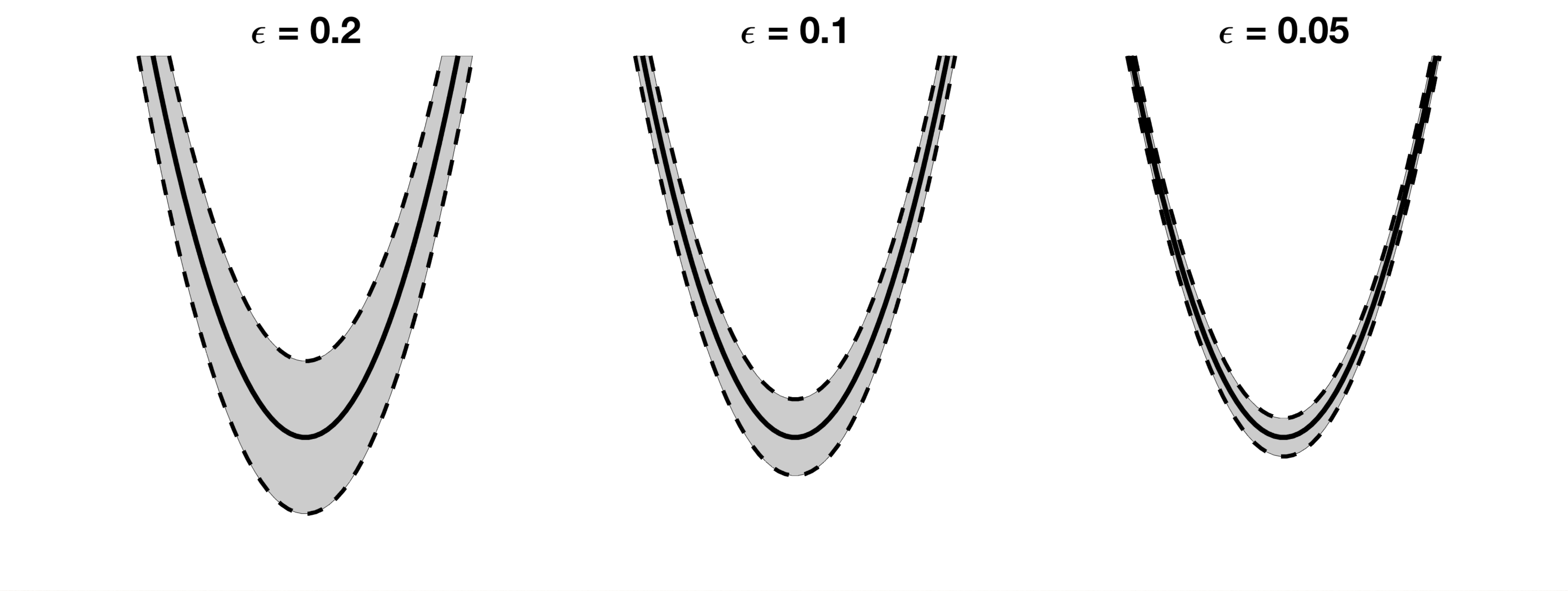
$q(x, y) = y - x^2$ $\qquad$ $M^\epsilon = \{(x, y) : -\epsilon < y - x^2 < \epsilon, \;\; y < 1\}$



(x(s),y(s)) = arc-length parameterization, $\sigma(ds) = ds$

Example

$$q(x, y) = y - x^2 \qquad M^\epsilon = \{(x, y) : -\epsilon < y - x^2 < \epsilon,\ \ y < 1\}$$



(x(s),y(s)) = arc-length parameterization, $\sigma(ds) = ds$

$$\rho^\epsilon(s) \approx (Z^\epsilon)^{-1} \frac{\epsilon}{|\nabla q(s)|} \implies \rho(s) \propto |\nabla q(s)|^{-1}$$

Coarea formula (formal)

e.g. Federer, (1959)

$$|\nabla q(x)|^{-1}\sigma(dx) = \delta(q(x))dx$$

i.e. $f(x) = |\nabla q(x)|^{-1}$

pseudo-determinant $\quad |\nabla q| = |(\nabla q)^T \nabla q|^{1/2}, \qquad \nabla q = (\nabla q_1 \;\; \nabla q_2 \;\; \cdots \nabla q_m)$

How to sample the measure $\rho(x) = Z^{-1} f(x) \sigma(dx)$?

- Give simple algorithm here (Zappa, H.-C., Goodman, CPAM 2018)
  Not necessarily the most efficient.
  But, the most efficient to program!
- For a Hamiltonian-based method, see e.g. T. Lelievre's talk
  - Lelievre, Rousset, Stoltz , arxiv (2018)
- Also:
  - Diaconis, Holmes, Shashahani, (2013)
  - Byrne, Girolami, Scan. J. Stat. (2013)
  - Cicotti, Vanden-Eijnden, Chem Phys Chem (2006)

Sampling algorithm. Generate random variables $X_1, X_2, \ldots$ via a random walk on M.

- Suppose $X_n = x$.
- Let T_x = Tangent space to M, at x

  N_x = Normal space to M, at x

  $$\mathbb{R}^n \text{ "=" } T_x \oplus N_x$$

- Propose $y = x + v + w$ with
  - $v \in T_x$ —> density $p(v;x)$
  - $w \in N_x$ —> solve $q(x+v+w) = 0$.

- Metropolis-Hastings accept/Reject move:

Acceptance probability $\min\left(1, \dfrac{f(y)T(y \to x)}{f(x)T(x \to y)}\right)$

$T(x \to y)\sigma(dy) =$ transition density on M

Sampling algorithm. Generate random variables $X_1, X_2, \ldots$ via a random walk on M.

- Suppose $X_n = x$.
- Let T_x = Tangent space to M, at x

  N_x = Normal space to M, at x

$$\mathbb{R}^n \text{ "=" } T_x \oplus N_x$$

Warning! Notation abuse!

T_x is also orthonormal matrix

- Propose $y = x + v + w$ with
  - $v \in T_x$ —> density $p(v;x)$
  - $w \in N_x$ —> solve $q(x+v+w) = 0$.

- Metropolis-Hastings accept/Reject move:

Acceptance probability $$\min\left(1, \frac{f(y)T(y \to x)}{f(x)T(x \to y)}\right)$$

$T(x \to y)\sigma(dy) =$ transition density on M

Sampling algorithm. Generate random variables $X_1, X_2, \ldots$ via a random walk on M.

- Suppose $X_n = x$.
- Let T_x = Tangent space to M, at x

  N_x = Normal space to M, at x

  $$\mathbb{R}^n \text{ "=" } T_x \oplus N_x$$

Warning! Notation abuse!

T_x is also orthonormal matrix

How to compute:

$QR(\nabla q) = (N_x \mid T_x) R$

- Propose $y = x + v + w$ with
  - $v \in T_x$ —> density $p(v;x)$
  - $w \in N_x$ —> solve $q(x+v+w) = 0$.

- Metropolis-Hastings accept/Reject move:

Acceptance probability $\min\left(1, \dfrac{f(y)T(y \to x)}{f(x)T(x \to y)}\right)$

$T(x \to y)\sigma(dy) =$ transition density on M

Sampling algorithm. Generate random variables $X_1, X_2, \ldots$ via a random walk on M.

- Suppose $X_n = x$.
- Let T_x = Tangent space to M, at x

  N_x = Normal space to M, at x

  $\mathbb{R}^n$ "=" $T_x \oplus N_x$

Warning! Notation abuse!

T_x is also orthonormal matrix

How to compute:

$QR(\nabla q) = (N_x \mid T_x) R$

- Propose $y = x + v + w$ with
  - $v \in T_x$ —> density $p(v;x)$
  - $w \in N_x$ —> solve $q(x+v+w) = 0$.

  Solve $q\left(x + v + \sum_{i=1}^{m} a_i \nabla q_i\right) = 0$ for $a=(a_1,\ldots,a_m)$.

- Metropolis-Hastings accept/Reject move:

  Acceptance probability $\min\left(1, \frac{f(y)T(y \to x)}{f(x)T(x \to y)}\right)$

  $T(x \to y)\sigma(dy) =$ transition density on M

Sampling algorithm. Generate random variables $X_1, X_2, \ldots$ via a random walk on M.

- Suppose $X_n = x$.
- Let T_x = Tangent space to M, at x

  N_x = Normal space to M, at x

  $\mathbb{R}^n$ "=" $T_x \oplus N_x$

Warning! Notation abuse!
T_x is also orthonormal matrix

How to compute:
$QR(\nabla q) = (N_x \mid T_x) R$

- Propose $y = x + v + w$ with
  - $v \in T_x$ —> density $p(v;x)$
  - $w \in N_x$ —> solve $q(x+v+w) = 0$.

  Solve $q\left(x + v + \sum_{i=1}^{m} a_i \nabla q_i\right) = 0$ for $a=(a_1,\ldots,a_m)$.

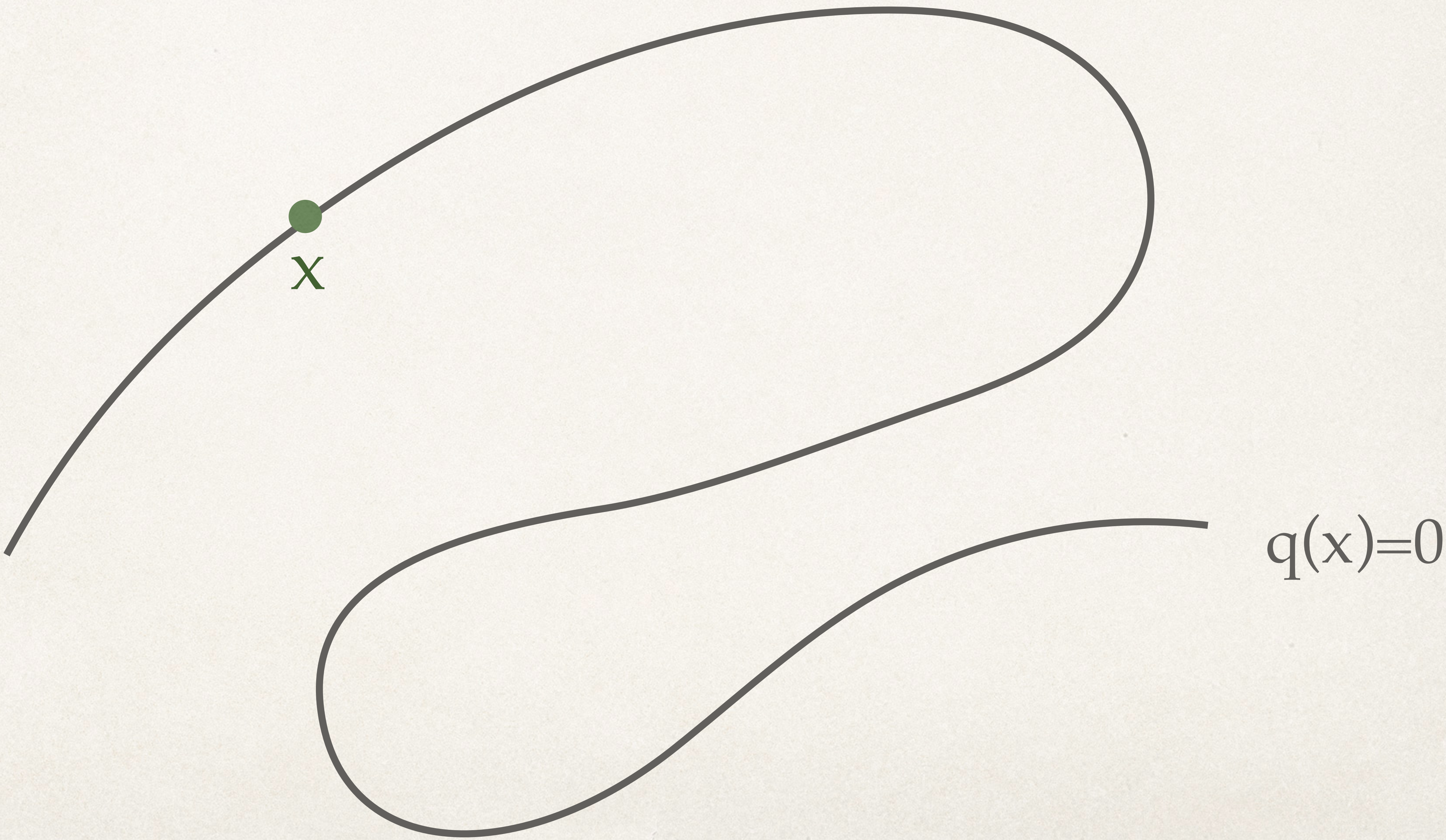
There are other ways to find w! (eg $w \in N_y$.)
But this one has a lot of nice properties.

- Metropolis-Hastings accept/Reject move:

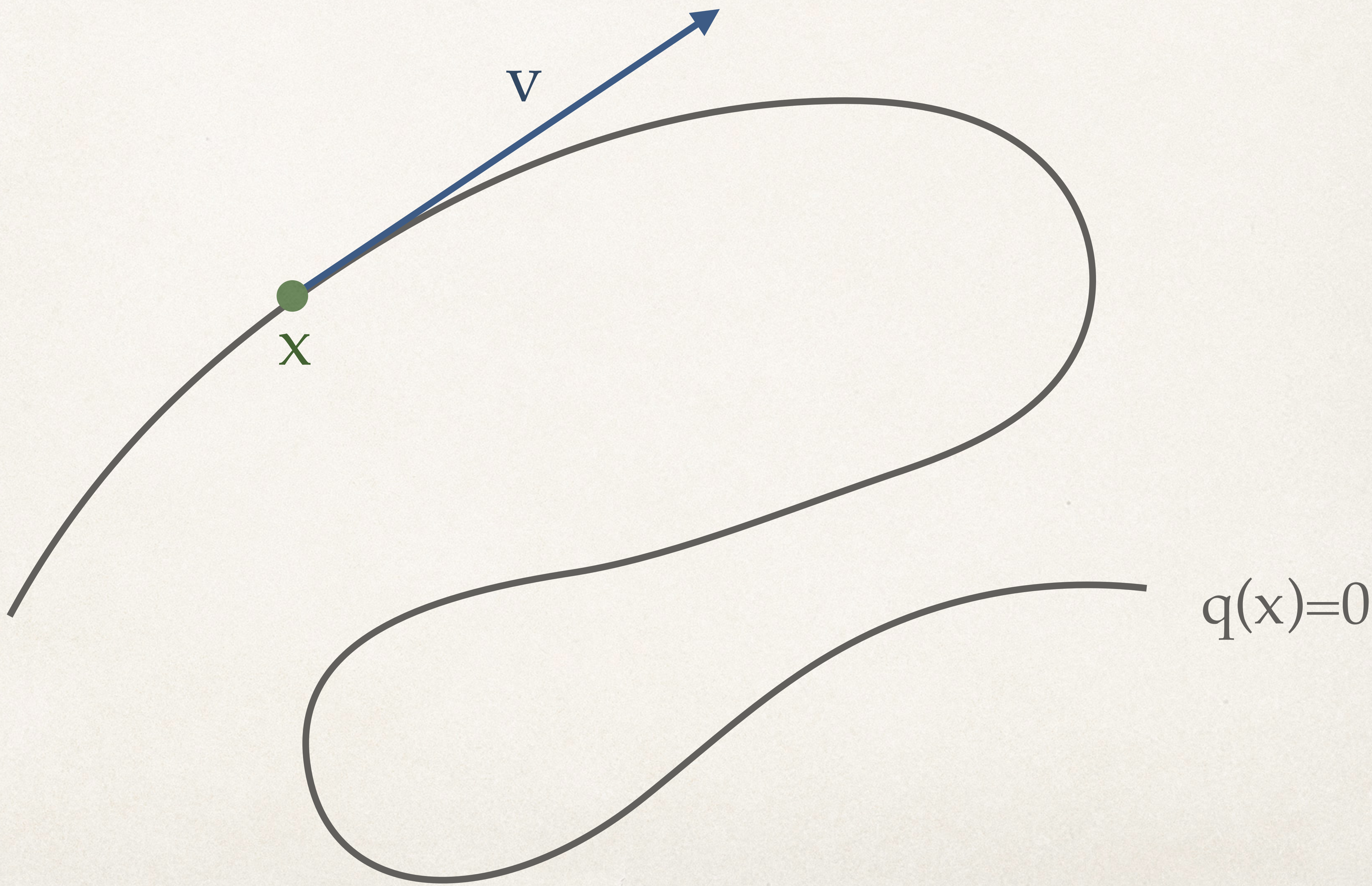
Acceptance probability $\min\left(1, \dfrac{f(y)T(y \to x)}{f(x)T(x \to y)}\right)$

$T(x \to y)\sigma(dy) =$
transition density on M

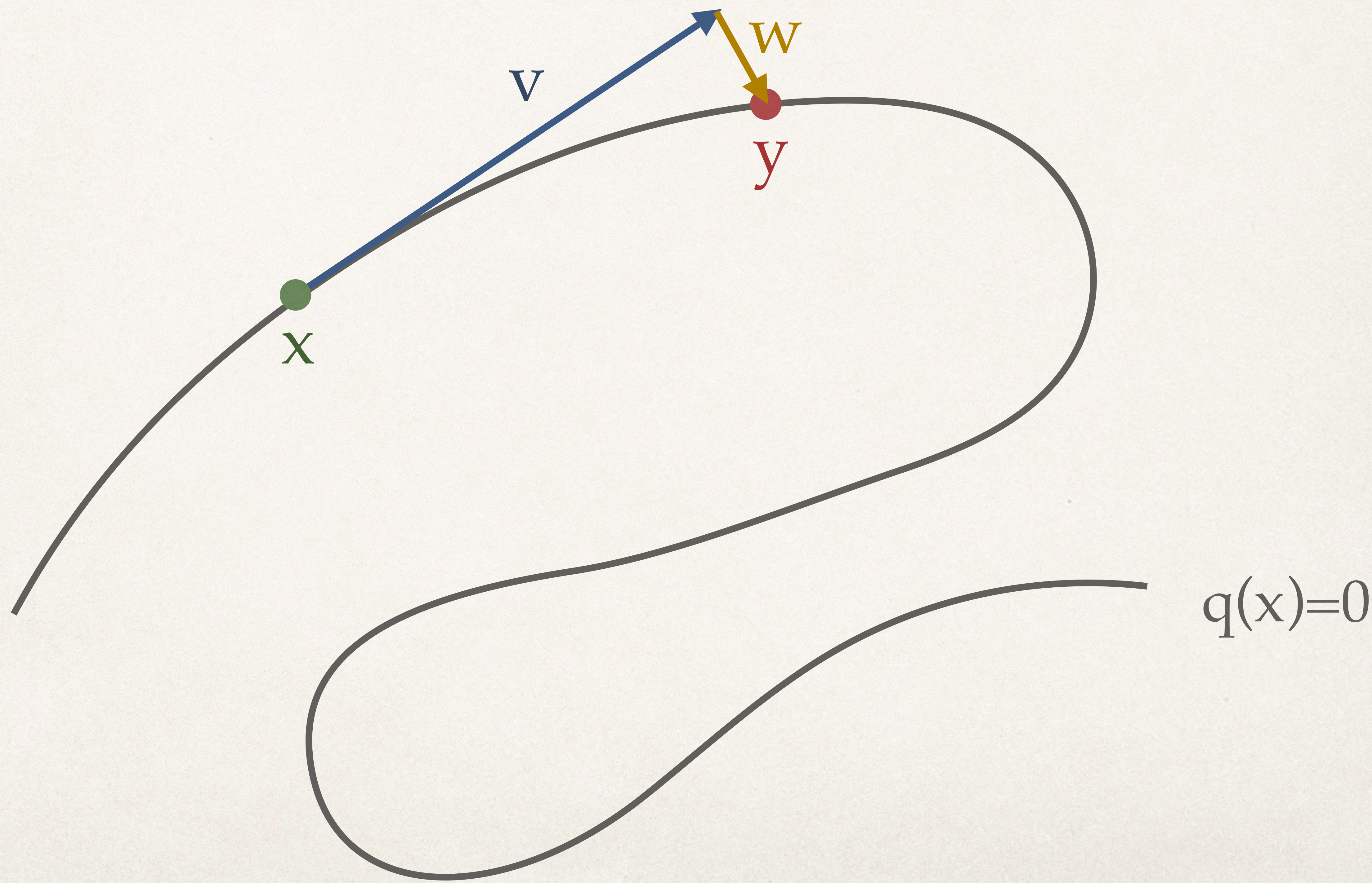
Proposal Move



Proposal Move



Proposal Move



Proposal densities $T(x \to y),\ T(y \to x)$

$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

$$\begin{aligned} p(v; x) &= \text{density of } v \text{ at } x \\ \left| \frac{\partial y}{\partial v} \right| &= \text{volume element for transformation } v \to y \\ A_x &= y \in M \text{ such that } y \text{ can be reached from } x \\ &\quad\ \text{using numerical solver} \\ \xi_x &= \text{probability of numerical solver failing} \\ &\quad\ \text{to find } y, \text{ after choosing } v \end{aligned}$$

Proposal densities $T(x \to y),\ T(y \to x)$

$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

density of v at x

Proposal densities $T(x \to y),\ \ T(y \to x)$

$$T(x \to y) = p(v;x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

density of v at x

$$\text{e.g.} \quad p(v;x) = \frac{1}{(2\pi s^2)^{d/2}} e^{-\frac{|v|^2}{2s^2}}$$

Proposal densities $\quad T(x \to y), \;\; T(y \to x)$

$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

density of v at x

e.g. $\quad p(v; x) = \frac{1}{(2\pi s^2)^{d/2}} e^{-\frac{|v|^2}{2s^2}}$

Reverse density

Proposal densities $T(x \to y), \;\; T(y \to x)$

$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

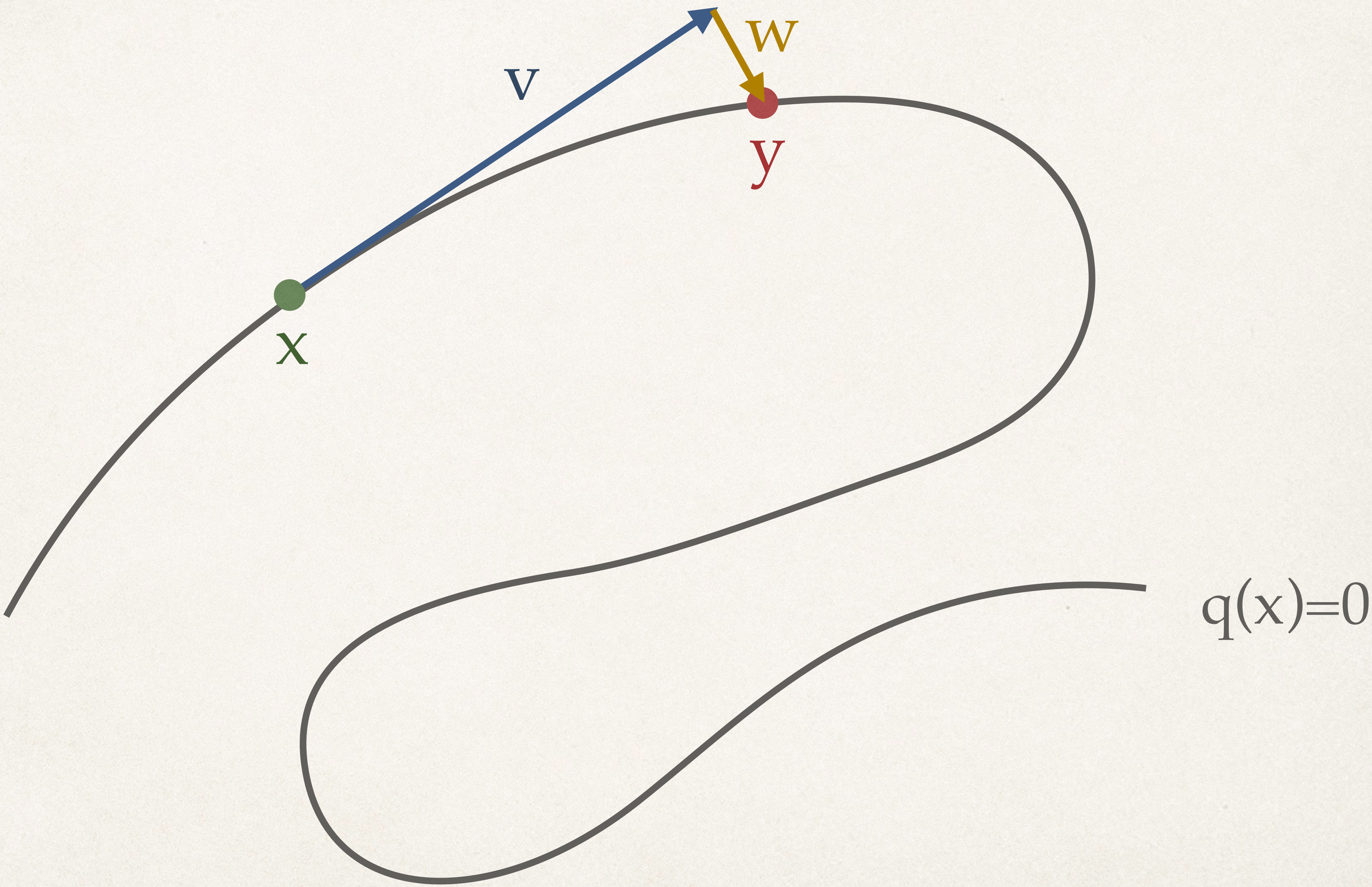
density of v at x

$$\text{e.g.} \quad p(v; x) = \frac{1}{(2\pi s^2)^{d/2}} e^{-\frac{|v|^2}{2s^2}}$$

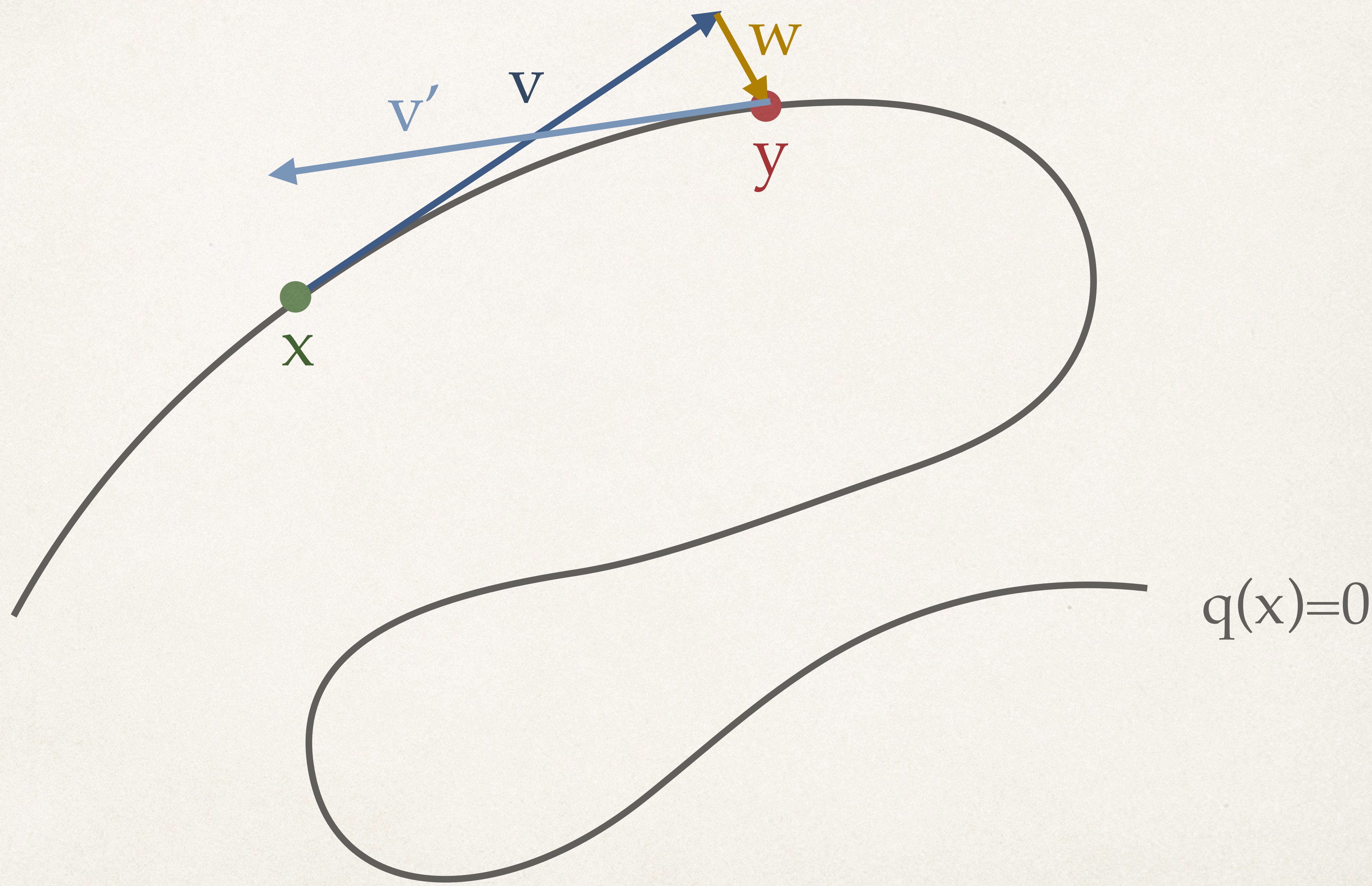
Reverse density

$$T(y \to x) = p(v'; y) \left| \frac{\partial x}{\partial v'} \right|^{-1} 1_{A_y}(x) \quad + \quad \xi_y \, \delta(x - y)$$

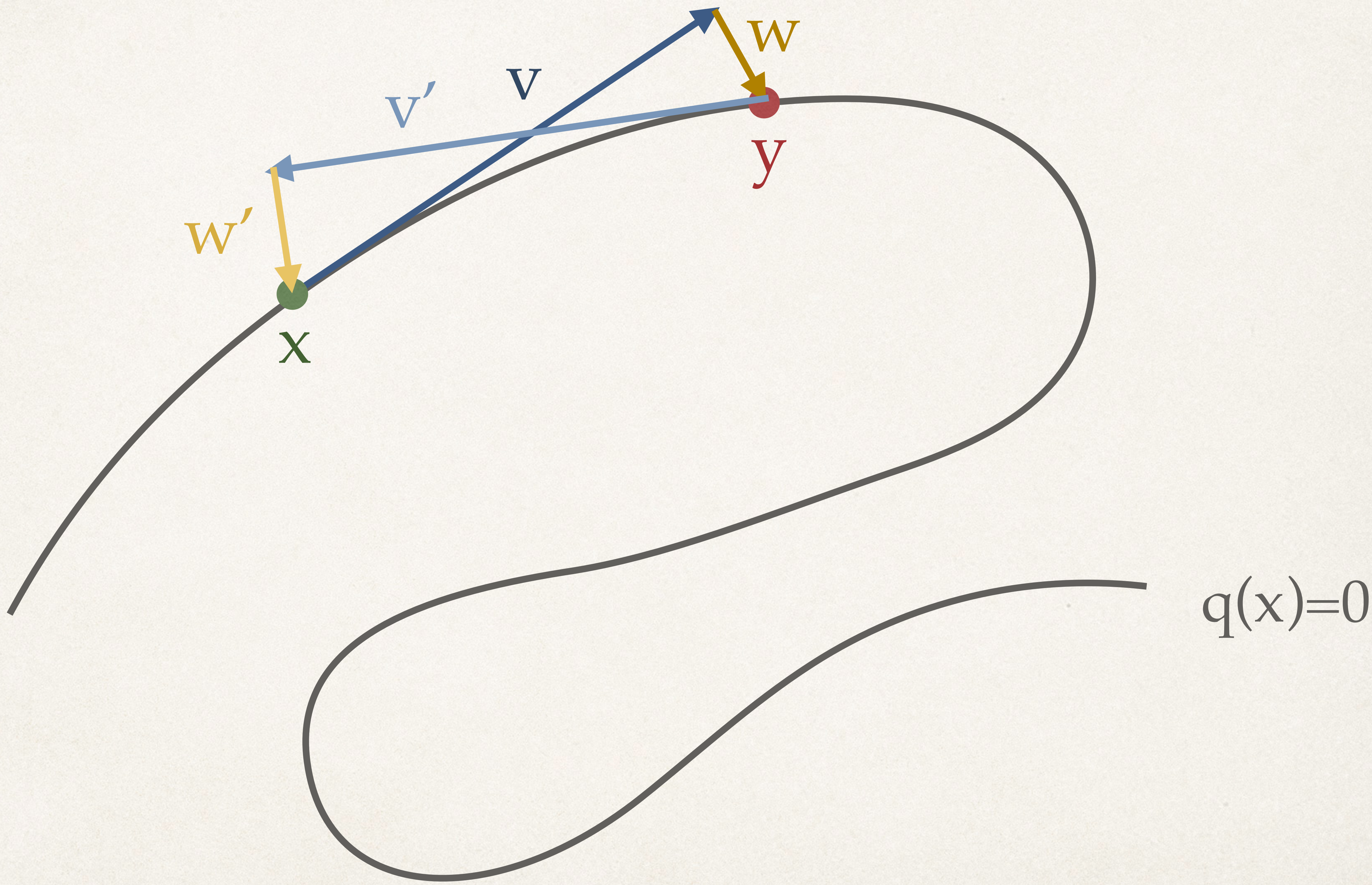
Proposal Move



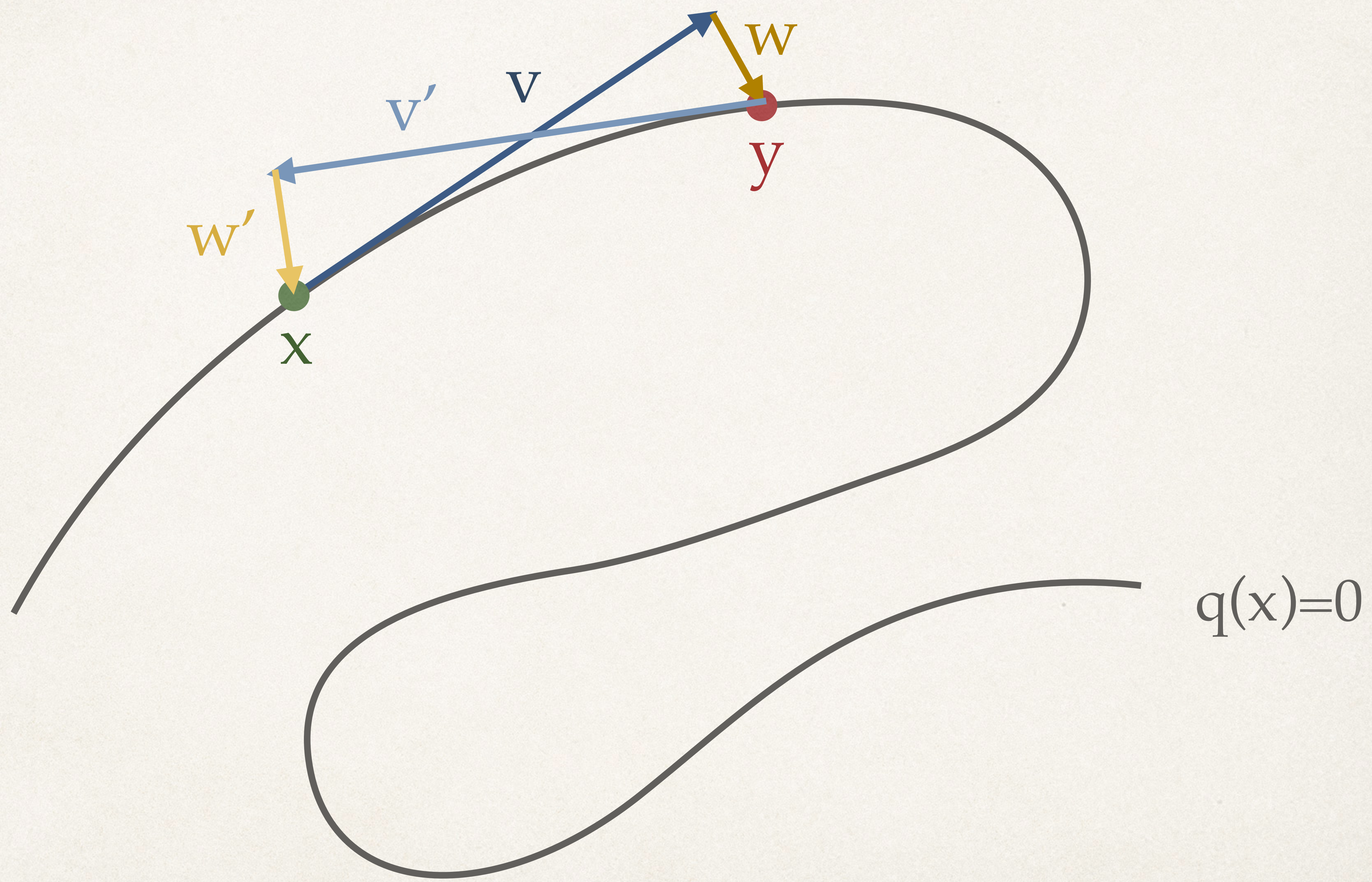
Proposal Move



Proposal Move



Proposal Move



$$v' = T_y T_y^T (x - y) \implies p(v'; x) \text{ is known}$$

Proposal densities $T(x \to y),\ T(y \to x)$

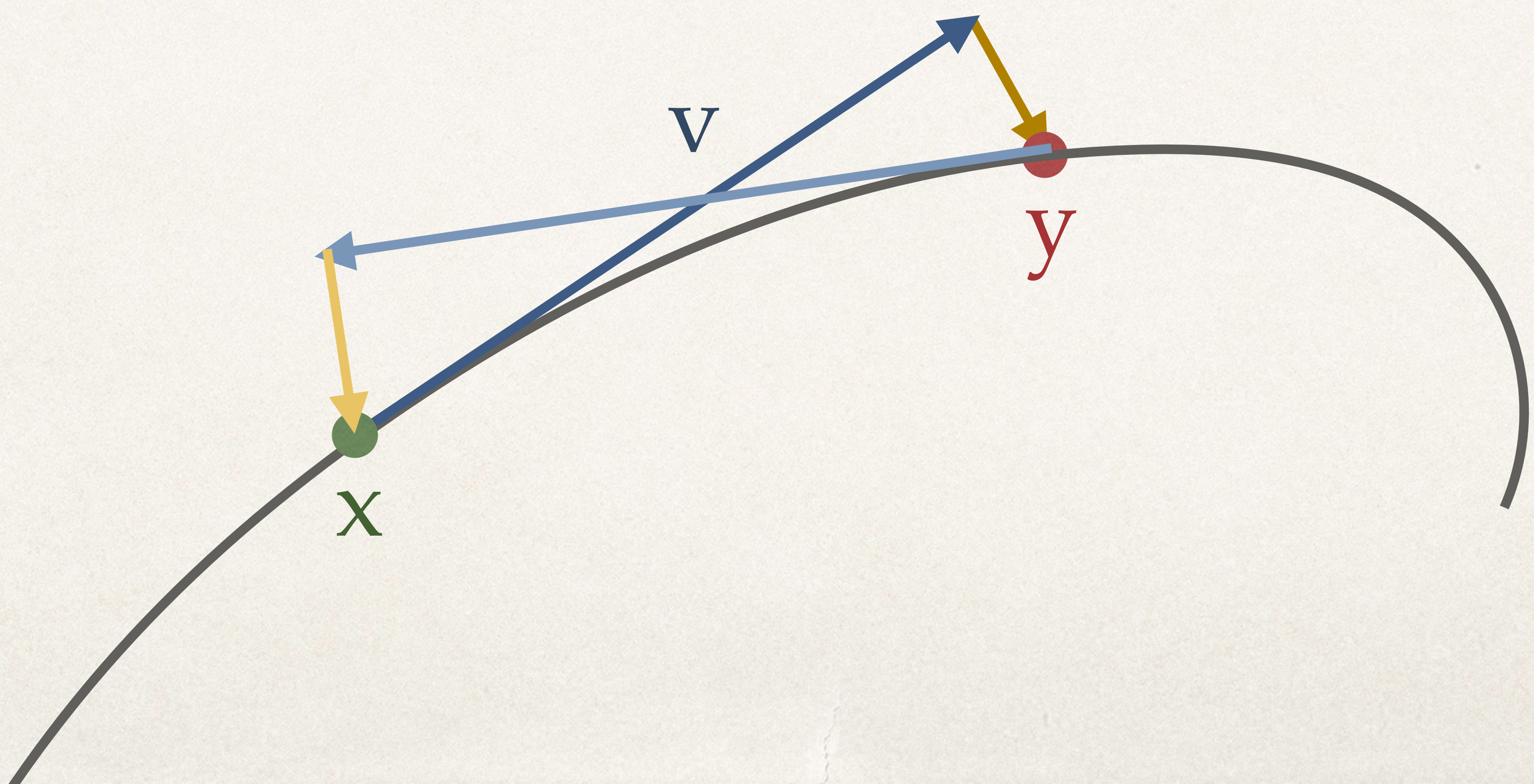
$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

volume element for transformation $v \to y$

Proposal densities $T(x \to y),\ T(y \to x)$

$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

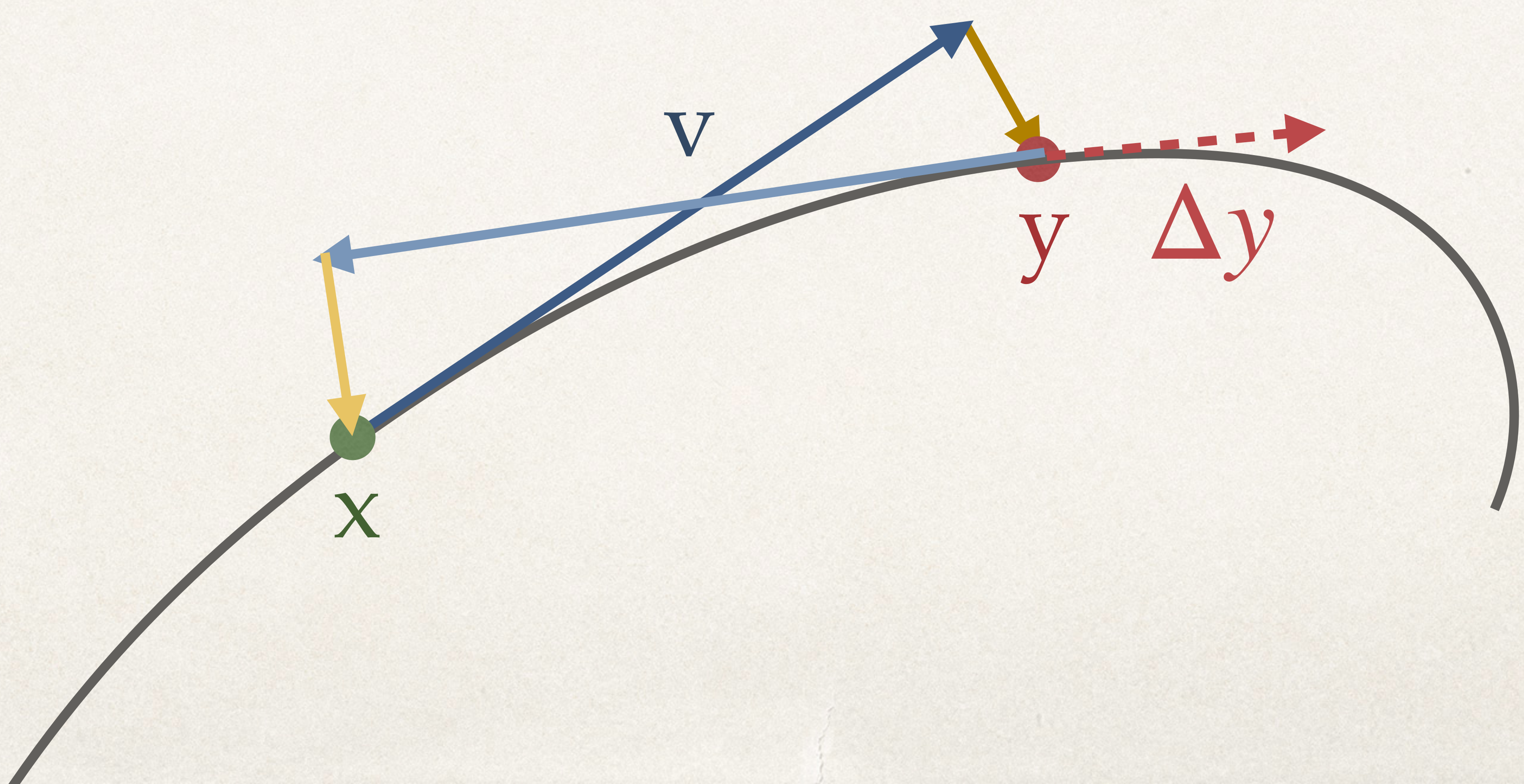
volume element for transformation $v \to y$



Proposal densities $T(x \to y),\ T(y \to x)$

$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

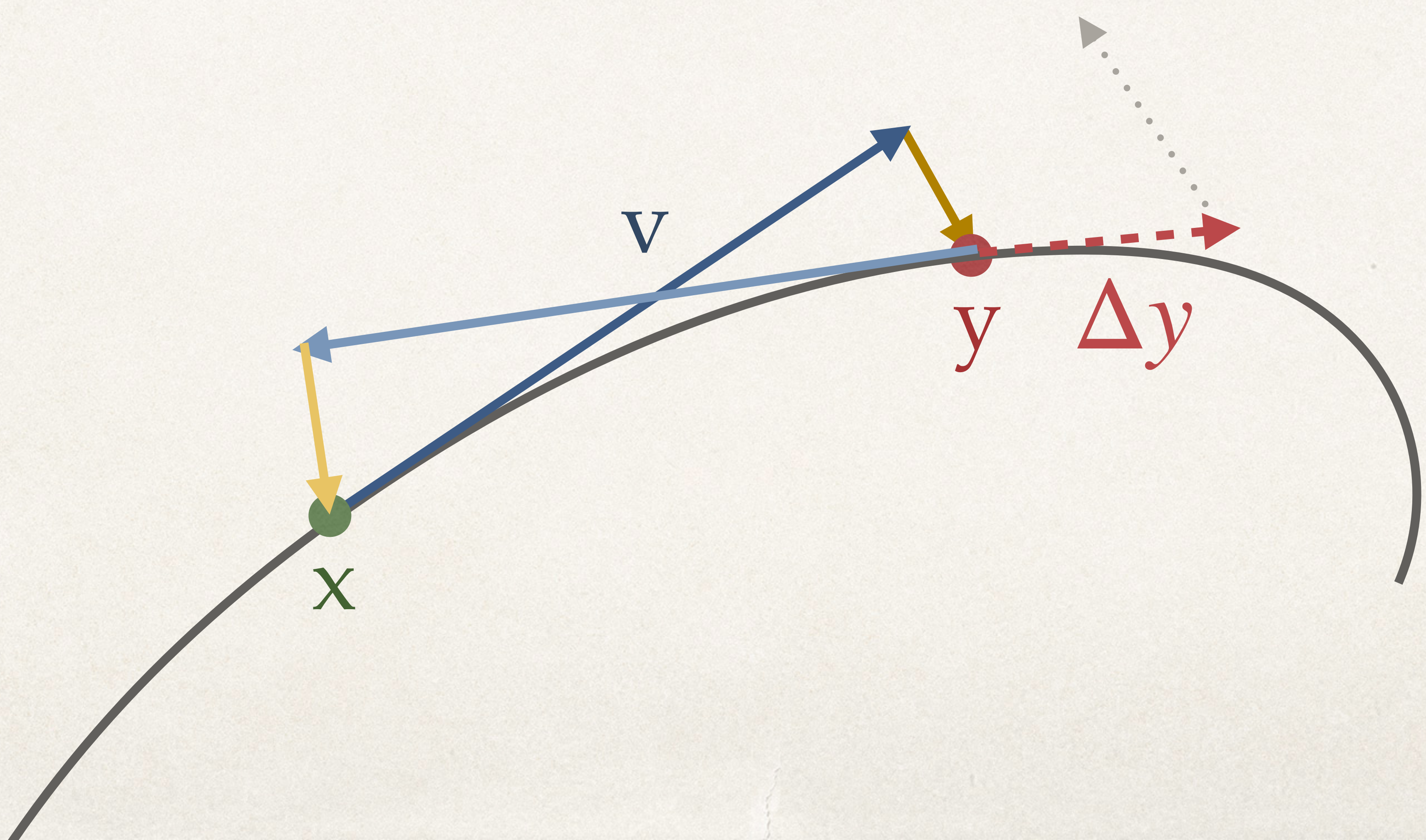
volume element for transformation $v \to y$



Proposal densities $T(x \to y),\ T(y \to x)$

$$T(x \to y) = p(v;x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x\, \delta(y - x)$$

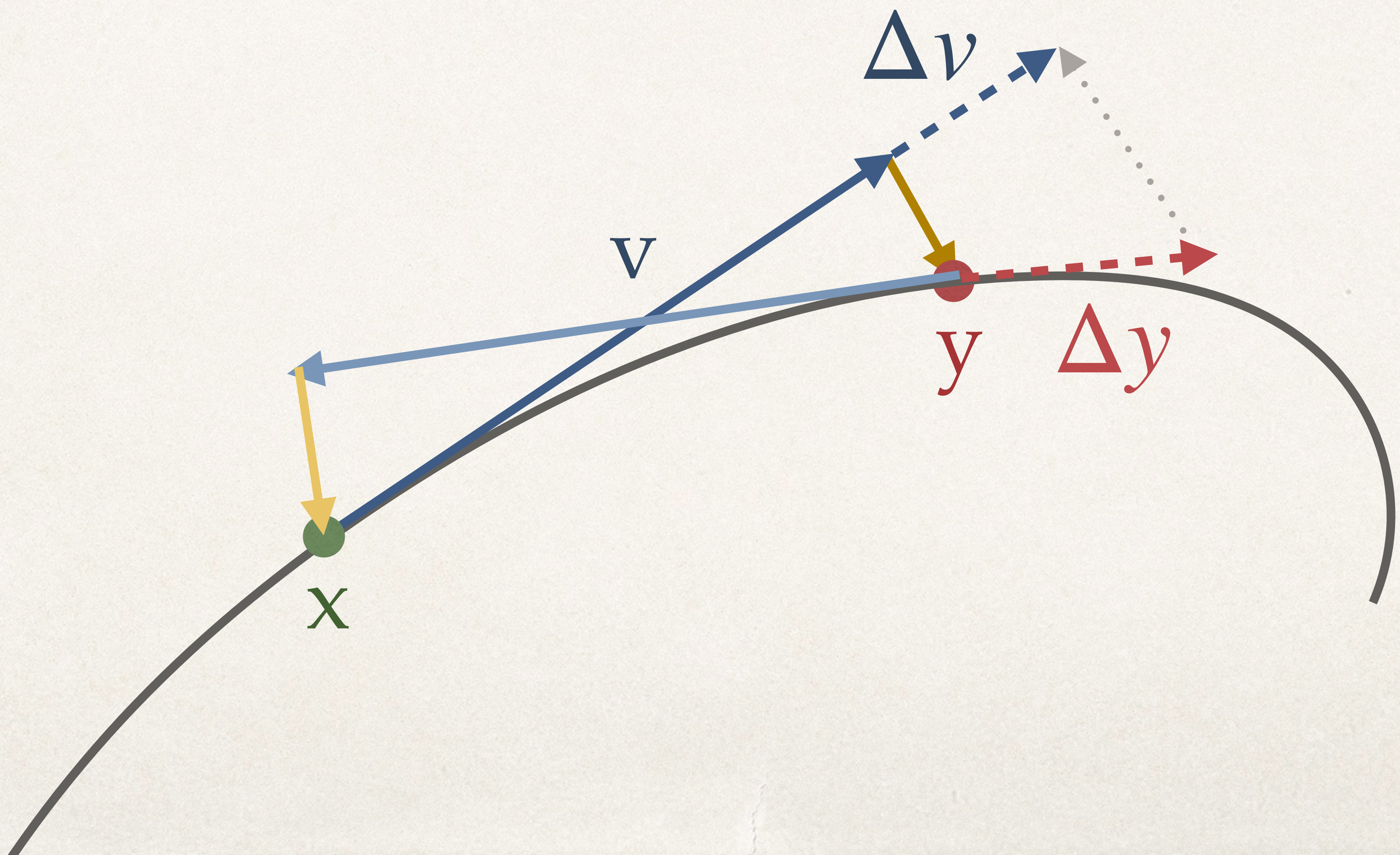
volume element for transformation $v \to y$



Proposal densities $T(x \to y), \;\; T(y \to x)$

$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \;\; + \;\; \xi_x \, \delta(y - x)$$

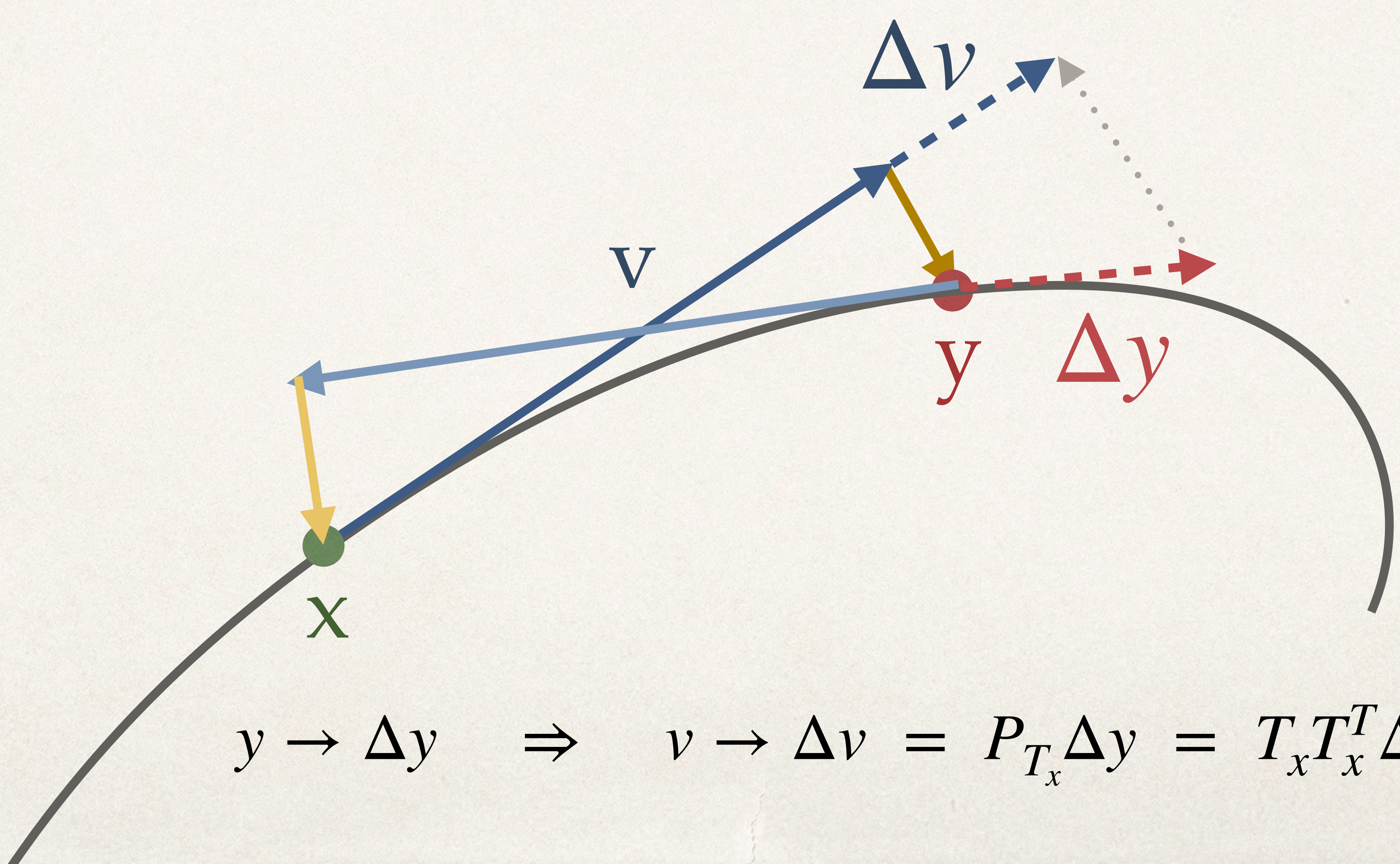
volume element for transformation $v \to y$



Proposal densities $T(x \to y),\ T(y \to x)$

$$T(x \to y) = p(v;x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \delta(y - x)$$

volume element for transformation $v \to y$



$$y \to \Delta y \quad \Rightarrow \quad v \to \Delta v \ = \ P_{T_x} \Delta y \ = \ T_x T_x^T \Delta y$$

$$\left| \frac{\partial y}{\partial v} \right|^{-1} = |T_x^T T_y|$$

$$\left|\frac{\partial y}{\partial v}\right|^{-1} = |T_x^T T_y|$$

...but...

$$\left|\frac{\partial x}{\partial v'}\right|^{-1} = |T_y^T T_x| \quad = \; |T_x^T T_y| \; !$$

Therefore these factors cancel, and we don't need to calculate them.

(Not true for stratifications...)

$$\left|\frac{\partial y}{\partial v}\right|^{-1} = |T_x^T T_y|$$

…but…

$$\left|\frac{\partial x}{\partial v'}\right|^{-1} = |T_y^T T_x| \quad = \; |T_x^T T_y| \; !$$

Therefore these factors cancel, and we don't need to calculate them.

(Not true for stratifications…)

If $w \in N_y$. these factors are much more complicated (and don't cancel.)

Proposal densities $T(x \to y),\ T(y \to x)$

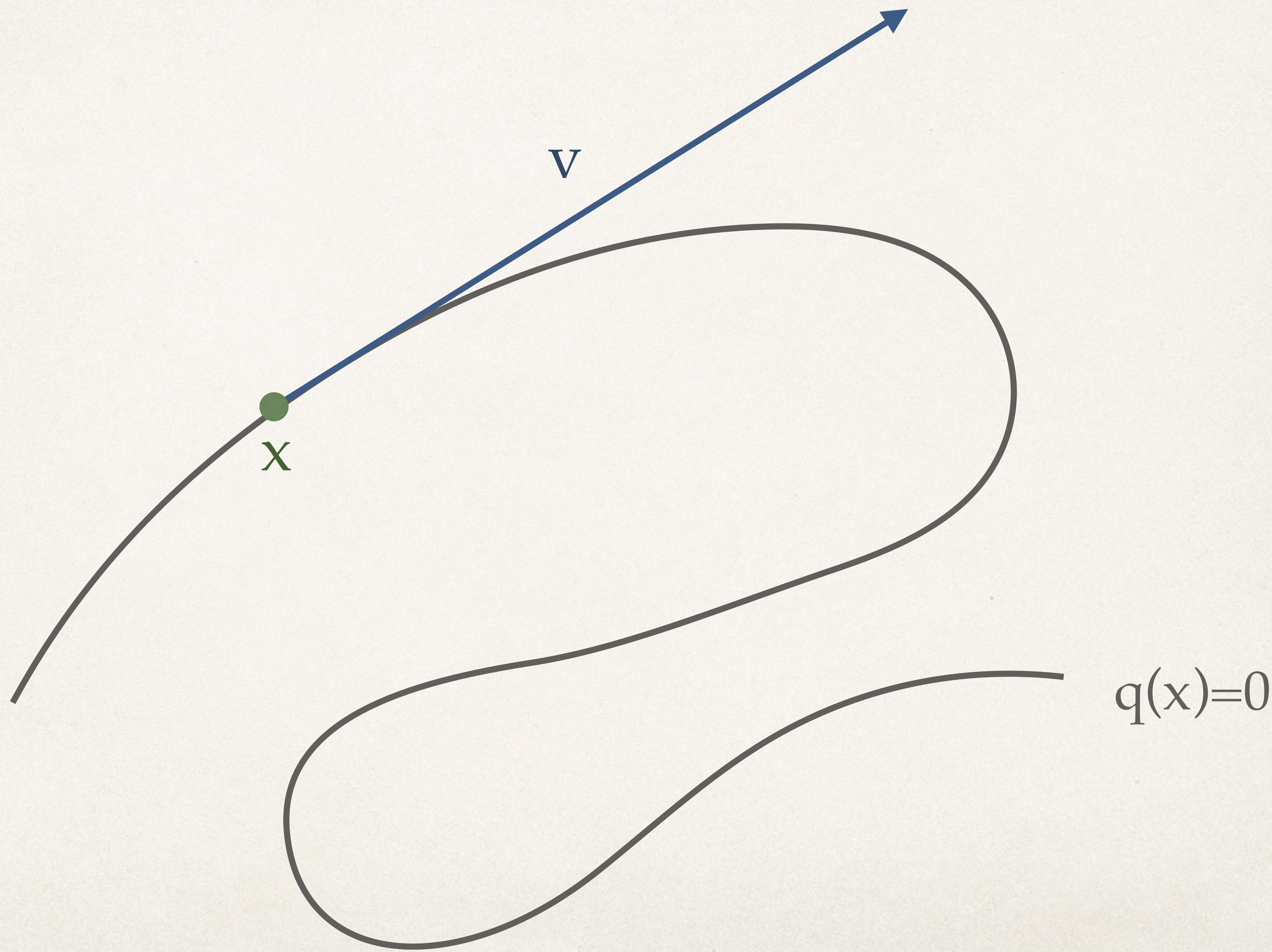
$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

$= 1$ if y can be reached from x using numerical solver

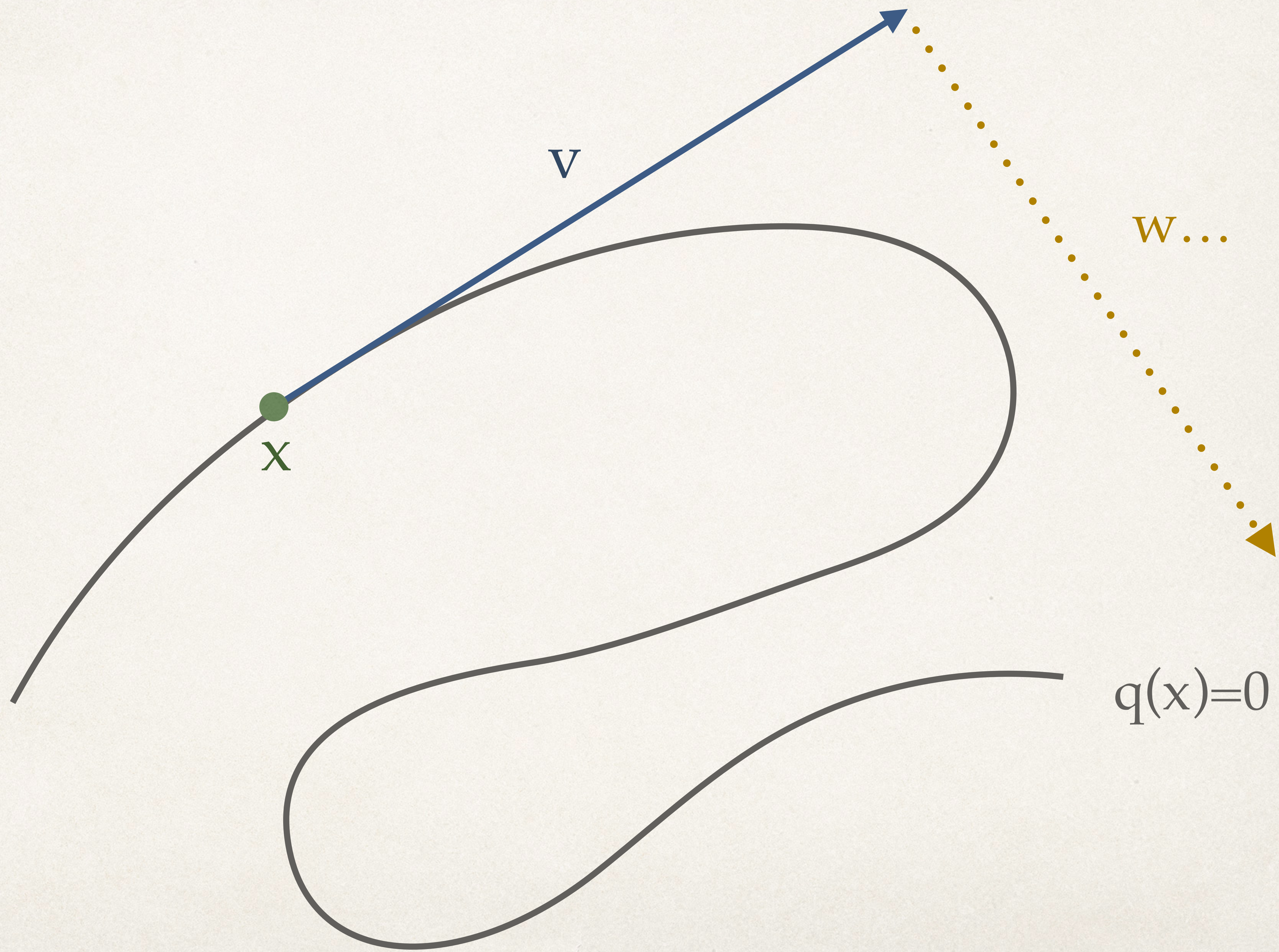
$= x$ if projection fails

What could go wrong?

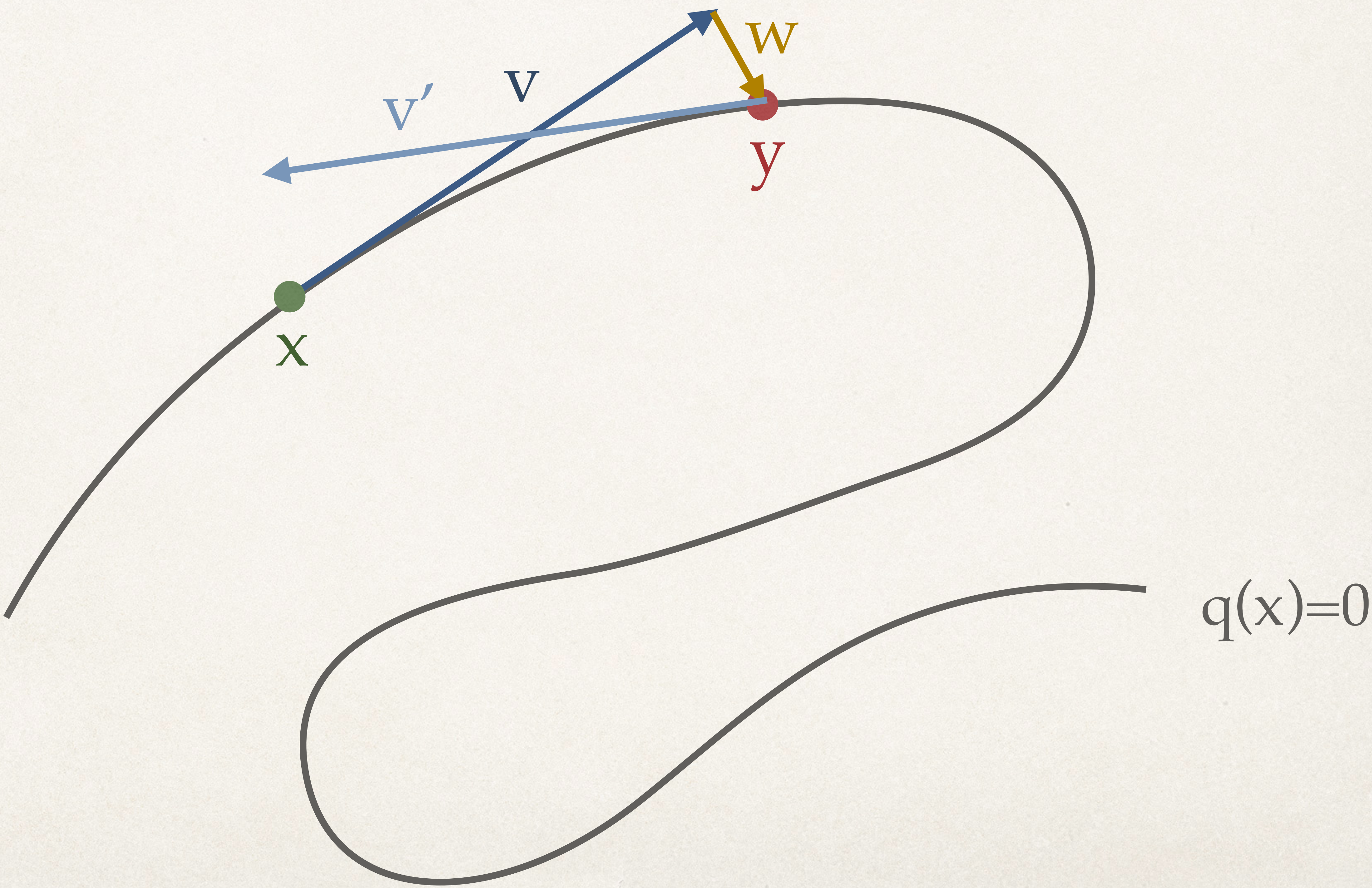
Solution doesn't exist (forward move)



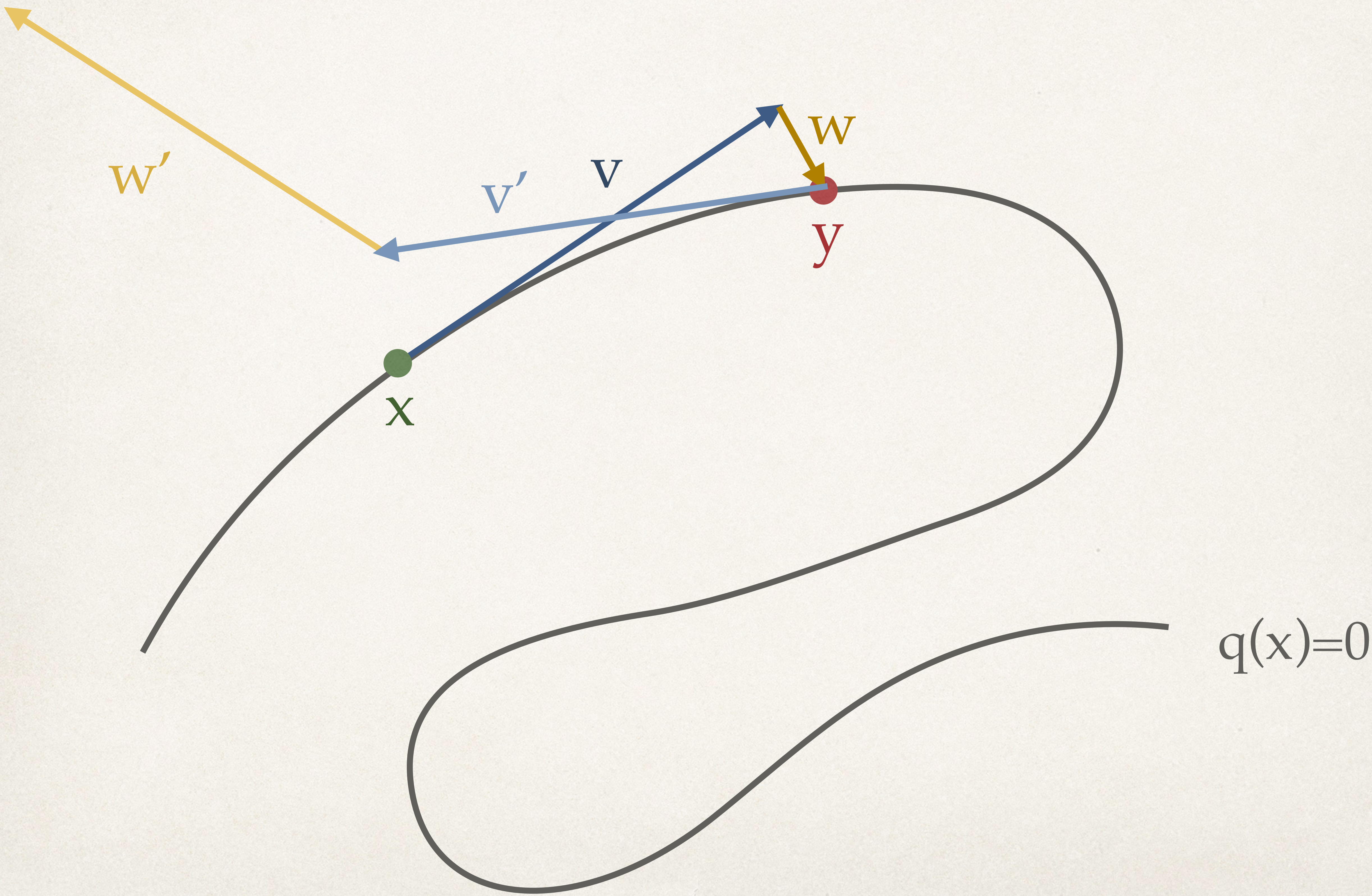
Solution doesn't exist (forward move)



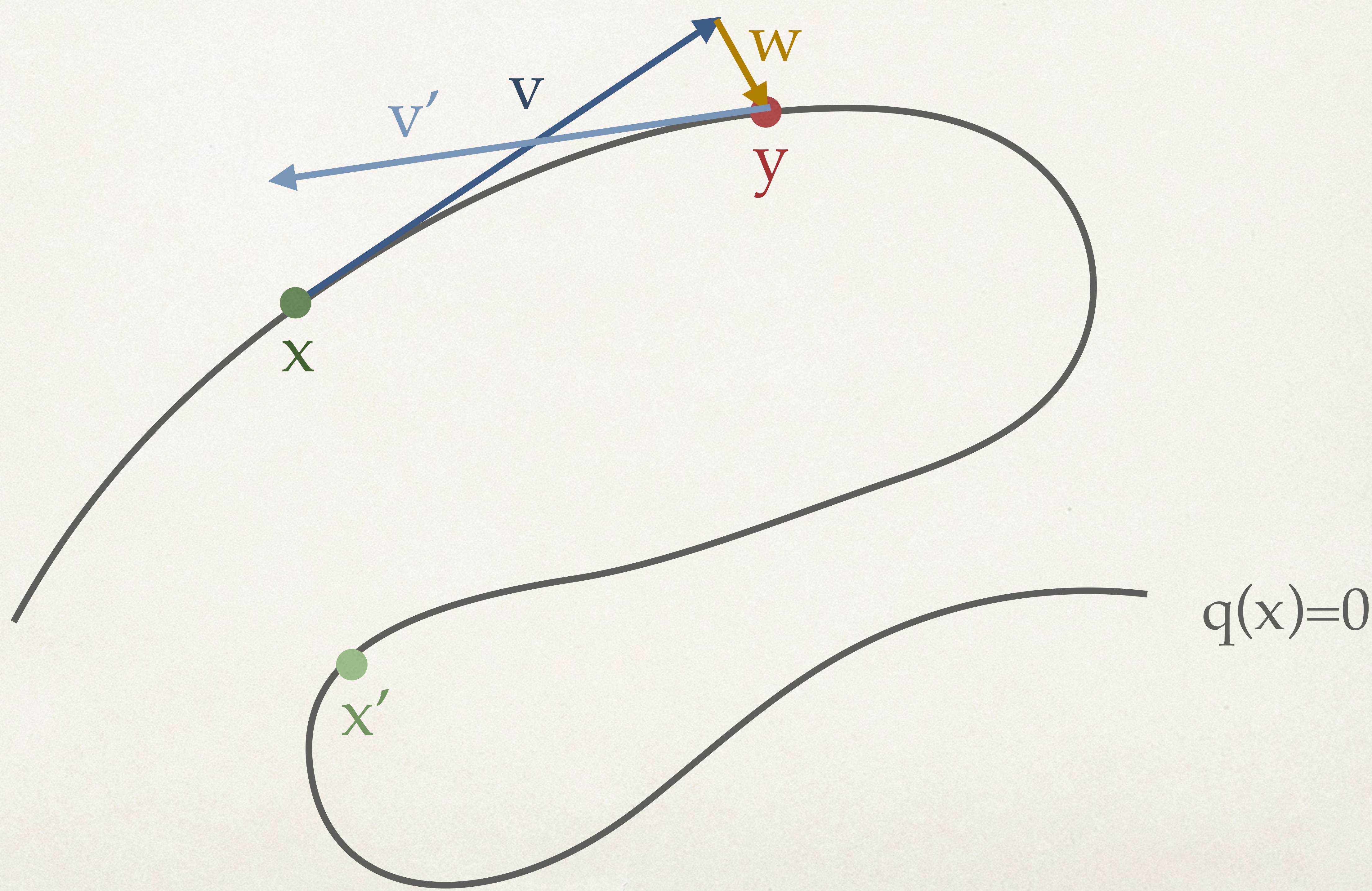
Numerical solver doesn't converge (forward & backward moves)



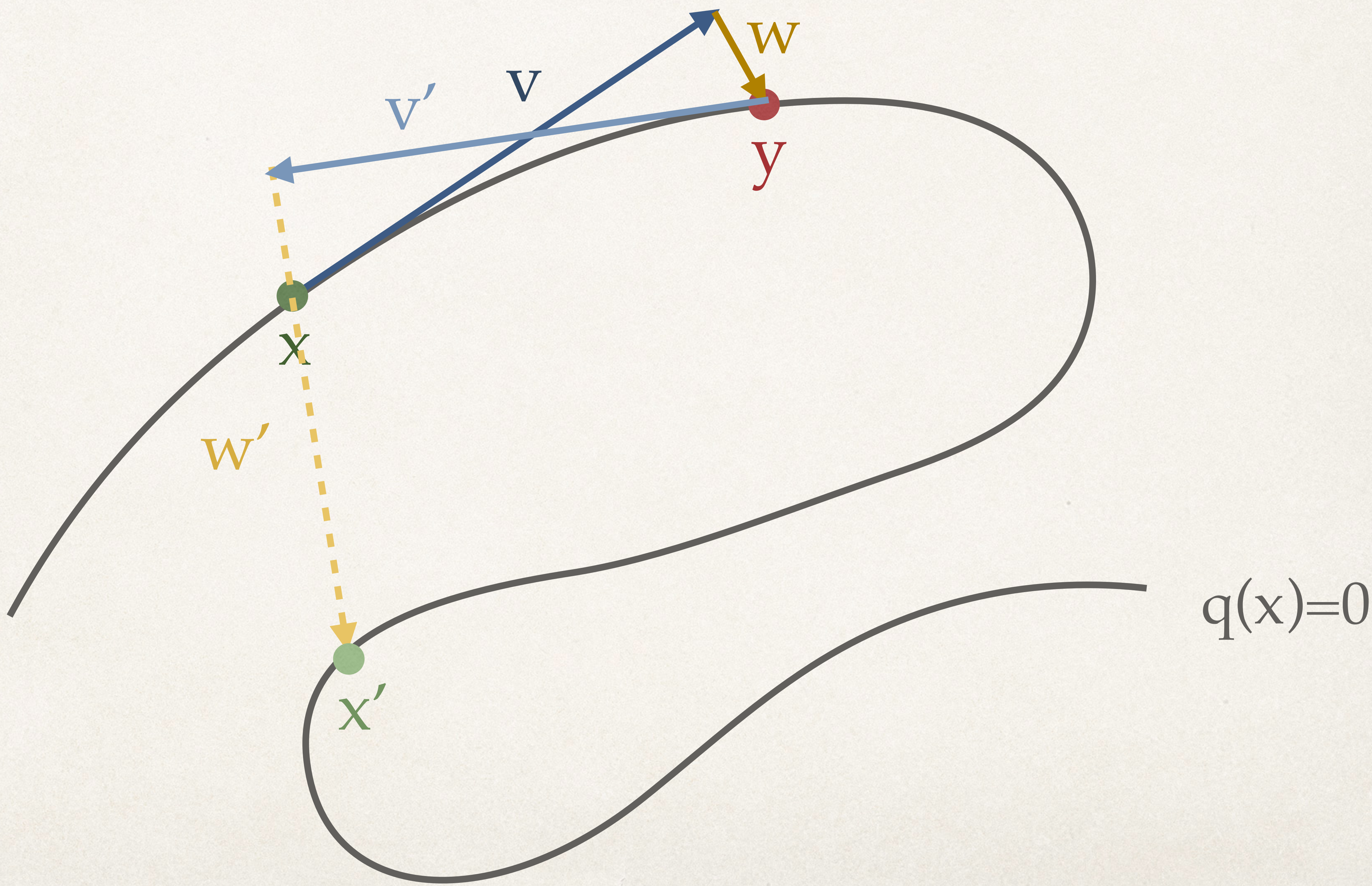
Numerical solver doesn’t converge (forward & backward moves)



Solver converges, but gives a different point x′ ≠ x (reverse move)



Solver converges, but gives a different point x′ ≠ x (reverse move)



Proposal densities $T(x \to y),\ T(y \to x)$

$$T(x \to y) = p(v; x) \left| \frac{\partial y}{\partial v} \right|^{-1} 1_{A_x}(y) \quad + \quad \xi_x \, \delta(y - x)$$

$= 1$ if y can be reached from x using numerical solver

$= x$ if projection fails

$$T(y \to x) = p(v'; y) \left| \frac{\partial x}{\partial v'} \right|^{-1} 1_{A_y}(x) \quad + \quad \xi_y \, \delta(x - y)$$

$= 1$ if x can be reached from y using numerical solver

$= y$ if projection fails

Given $y \in A_x$, we *don't know* if $x \in A_y$

—> **we have to check reverse projection**

Check: (i) reverse projection converges, (ii) it converges to x.

Code time!

Issues

- $|\nabla q| = 0$ —> then what?
- Is this really worth it? Projections are costly…
- Numerical solver — better to be lazy. How lazy?
- Can we sample a density concentrated near, but not exactly on, a manifold, using a similar technique?
- Numerically we are never exactly on the manifold… so why do we get the right measure?
- Inequalities & highly nonconvex spaces (can we treat them like constraints?)