EE613 - Machine Learning for Engineers

LINEAR REGRESSION

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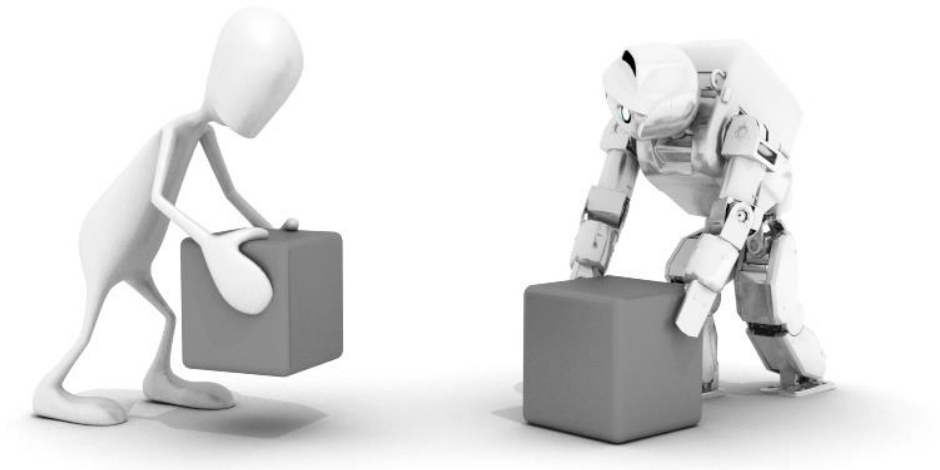
Sep 30, 2021

Robot Learning and Interaction group

Idiap Research Institute



Learning from demonstration

EE613 labs (INM11):

Dr João Silvério

Outline

Linear regression (Sep 30)

- Least squares
- Singular value decomposition (SVD)
- Nullspace projection (kernels in least squares)
- Ridge regression (Tikhonov regularization)
- Weighted least squares
- Iteratively reweighted least squares (IRLS)
- Recursive least squares
- Logistic regression

Tensor regression (Oct 7)

- Tensor factorization
- Tensor-variate regression

Nonlinear regression (Oct 14)

- Locally weighted regression (LWR)
- Gaussian mixture regression (GMR)
- Gaussian process regression (GPR)

Hidden Markov model (HMM) (Nov 11)

Regression

Nonlinear regression:

Approximation function
(predictor function)
(forecasting function)

$$y = f(x)$$

Output
(response variable)
(outcome variable)

Input
(explanatory variable)
(feature variable)

$\in \mathbb{R}$

Linear regression:

$$y = Ax$$

Tensor regression:

Similar to $y = Ax$, but with x a tensor instead of a vector

Nonlinear regression on x reformulated as linear regression on f:

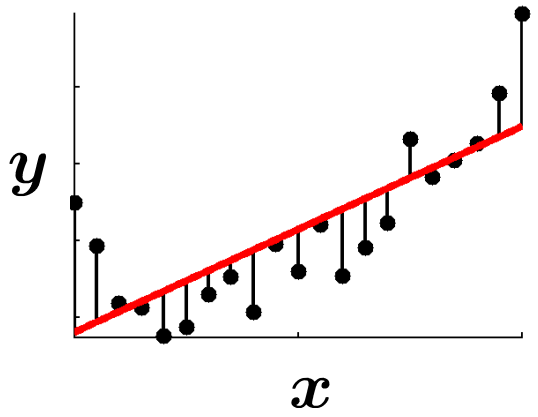
$$y = A \begin{bmatrix} f_1(x) \\ f_2(x) \\ \vdots \end{bmatrix}$$

LEAST SQUARES

circa 1795

Least squares: a ubiquitous tool

$$\hat{A} = X^{\dagger} Y$$



Weighted least squares?

Regularized least squares?

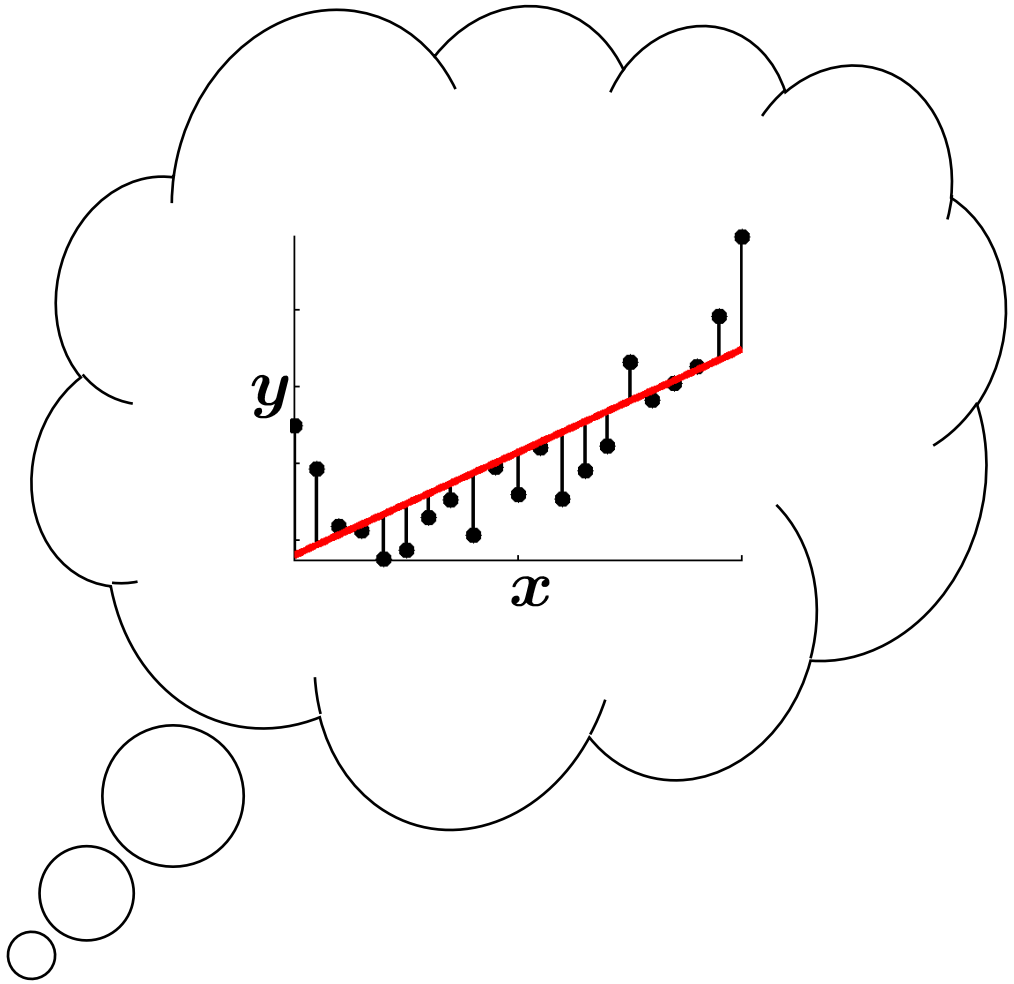
L1-norm instead of L2-norm?

Solution with a secondary objective?

Fast and robust implementation?

Recursive computation?

Youtube search for "deep learning regression"



YouTube CH

deep learning regression

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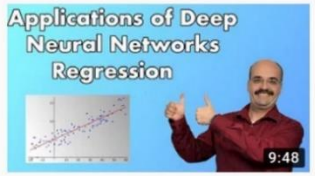


5.3: Regression Neural Networks for Keras and TensorFlow (Module 5, Part 3)

Jeff Heaton • 6K views • 1 year ago

Performing **regression** with keras **neural networks**. Producing a lift chart. This video is part of a course that is taught in a hybrid ...

Linear Regression Machine Learning (tutorial)

Siraj Raval • 87K views • Streamed 2 years ago

I'll perform linear **regression** from scratch in Python using a method called 'Gradient Descent' to determine the relationship ...

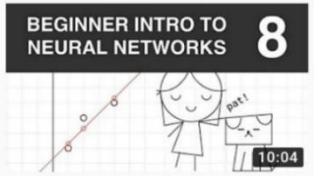
CC

3.4: Linear Regression with Gradient Descent - Intelligence and Learning

The Coding Train • 64K views • 1 year ago

In this video I continue my Machine Learning series and attempt to explain Linear Regression with Gradient Descent. My Video ...

CC



Beginner Intro to Neural Networks 8: Linear Regression

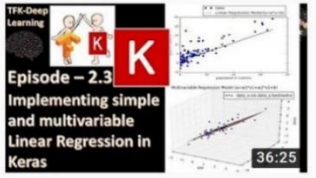
giant_neural_network • 53K views • 1 year ago

Hey everyone! In this video we're going to look at something called linear **regression**. We're really just adding an input to our ...

Learning Tensorflow with linear regression

Technology for Noobs • 3.5K views • 1 year ago

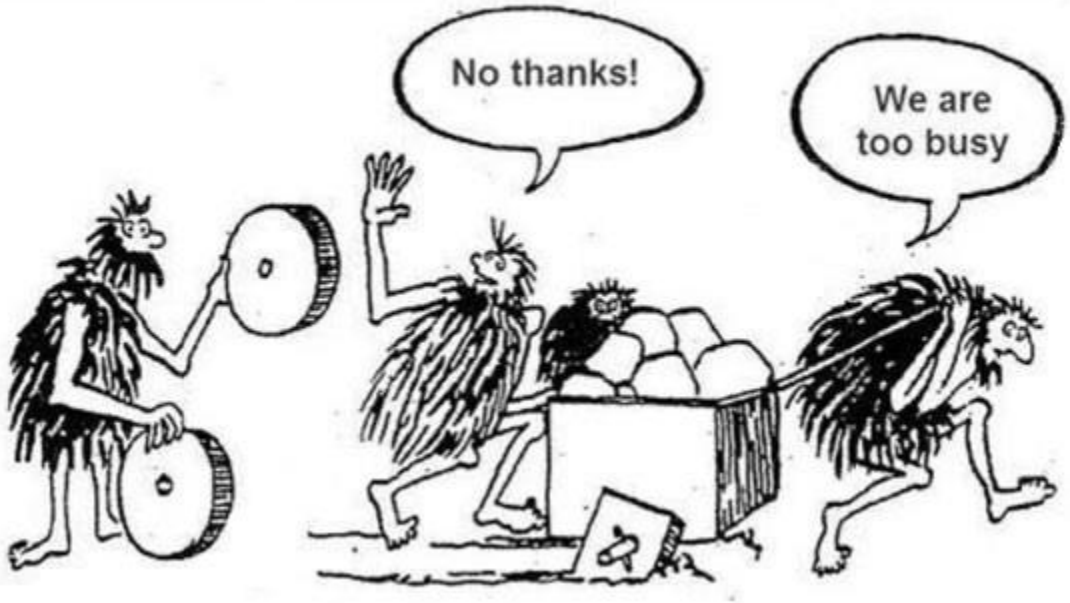
In this video, I will cover basics of tensorflow. Below are the topics that will be covered: 1. Basic of linear **regression** 2. Basics of ...



Ep-2.3: Linear Regression in Keras || TFK-Deep Learning || Exploring Neurons

Anuj shah • 1.2K views • 1 year ago

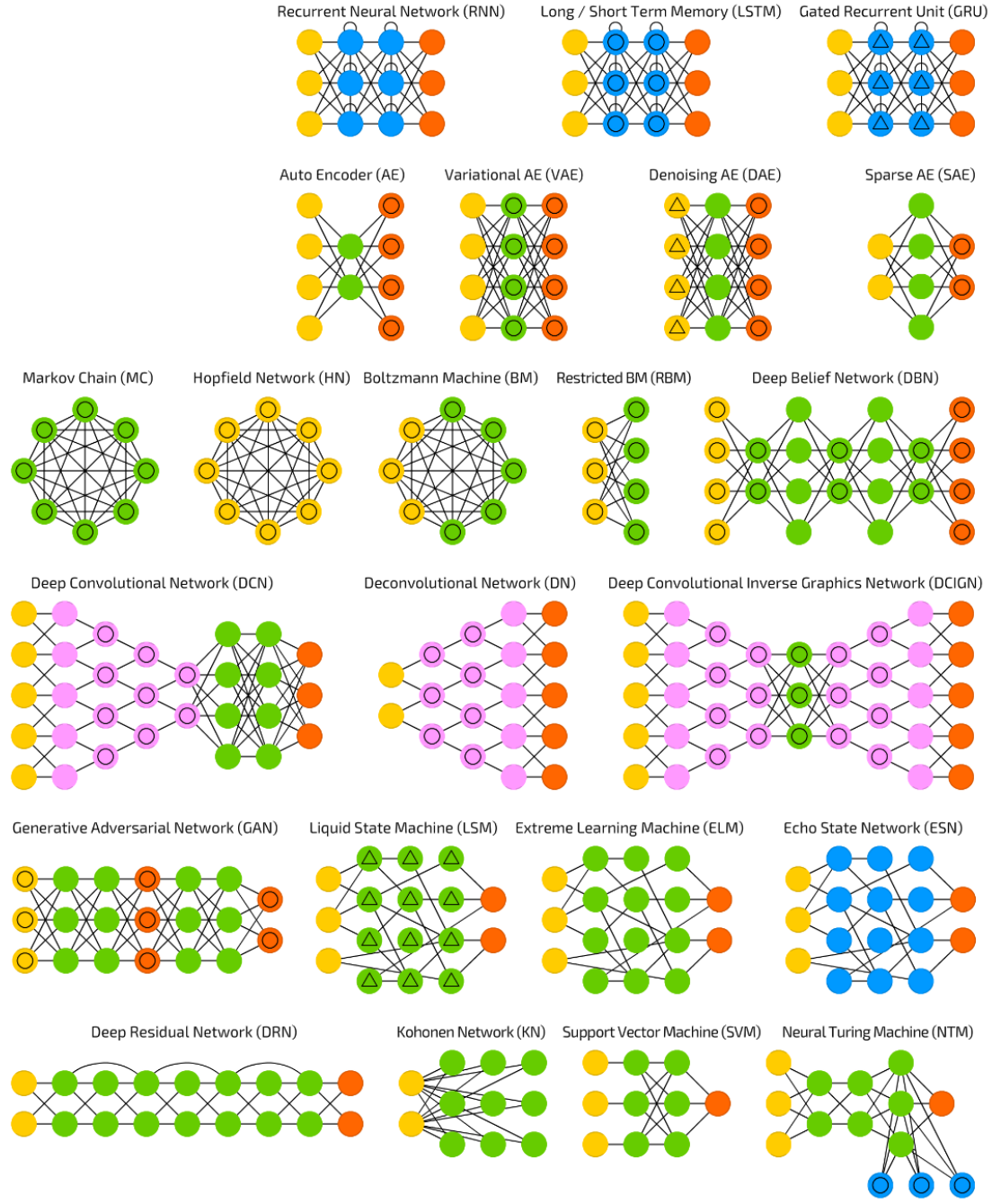
This video explains the implementation of simple and multiple linear **regression** in keras. The theoretical discussion of linear ...



The **pinv-net!** ☺
single layer,
single node,
linear activation!

$$\hat{A} = X^{\dagger} Y$$

- Backfed Input Cell
- Input Cell
- Noisy Input Cell
- Hidden Cell
- Probablistic Hidden Cell
- Spiking Hidden Cell
- Output Cell
- Match Input Output Cell
- Recurrent Cell
- Memory Cell
- Different Memory Cell
- Kernel
- Convolution or Pool

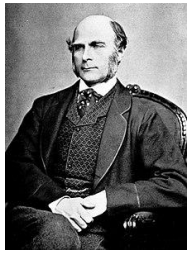


Multivariate linear regression (ordinary least squares)

- **Least squares is everywhere**: from simple problems to large scale problems.
- It was the earliest form of regression, which was published by **Legendre** in 1805 and by **Gauss** in 1809. They both applied the method to the problem of determining the orbits of bodies around the sun from astronomical observations.
- The term regression was only coined later by **Galton** to describe the biological phenomenon that the heights of descendants of tall ancestors tend to regress down towards a normal average.
- **Pearson** later provided the statistical context showing that the phenomenon is more general than a biological context.

Adrien-Marie Legendre

Carl Friedrich Gauss

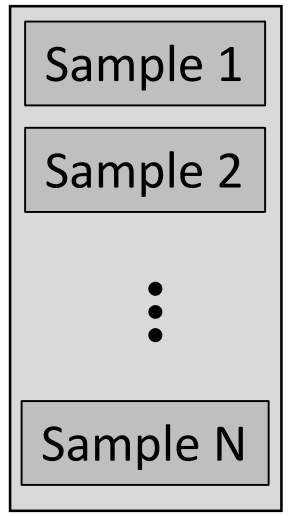


Francis Galton

Karl Pearson

Multivariate linear regression

By describing the input data as $\boldsymbol{X} \in \mathbb{R}^{N \times D^{\mathcal{I}}}$ and the output data as $\boldsymbol{y} \in \mathbb{R}^{N}$, we want to find $\boldsymbol{a} \in \mathbb{R}^{D^{\mathcal{I}}}$ to have $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{a}$.



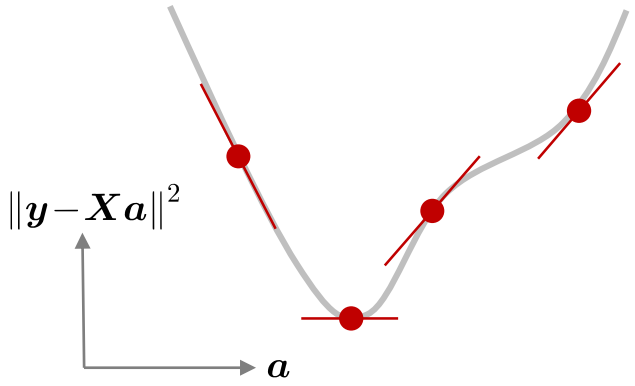
A solution can be found by minimizing the ℓ_2 norm

$$\begin{aligned}\hat{\boldsymbol{a}} &= \arg\min_{\boldsymbol{a}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{a}\|^2 \\ &= \arg\min_{\boldsymbol{a}} (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{a})^\top (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{a}) \\ &= \arg\min_{\boldsymbol{a}} \boldsymbol{y}^\top \boldsymbol{y} - 2\boldsymbol{a}^\top \boldsymbol{X}^\top \boldsymbol{y} + \boldsymbol{a}^\top \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{a}.\end{aligned}$$

By differentiating with respect to $\boldsymbol{a}$ and equating to zero

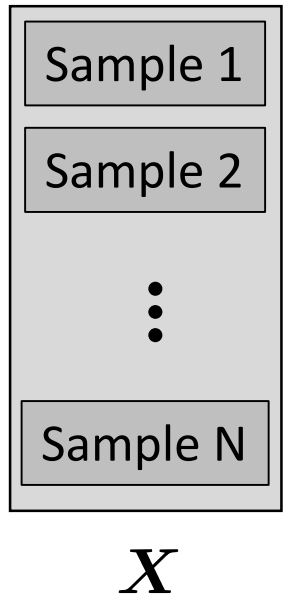
$$-2\boldsymbol{X}^\top \boldsymbol{y} + 2\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{a} = \boldsymbol{0} \quad \Longleftrightarrow \quad \hat{\boldsymbol{a}} = \left(\boldsymbol{X}^\top \boldsymbol{X}\right)^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

Moore-Penrose pseudoinverse $\boldsymbol{X}^\dagger$



Multiple multivariate linear regression

By describing the input data as $\boldsymbol{X} \in \mathbb{R}^{N \times D^{\mathcal{I}}}$ and the output data as $\boldsymbol{Y} \in \mathbb{R}^{N \times D^{\mathcal{O}}}$, we want to find $\boldsymbol{A} \in \mathbb{R}^{D^{\mathcal{I}} \times D^{\mathcal{O}}}$ to have $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{A}$.



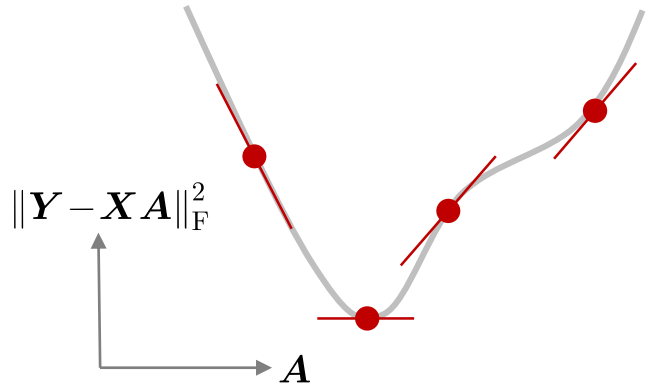
A solution can be found by minimizing the Frobenius norm

$$\begin{aligned}\hat{\boldsymbol{A}} &= \arg\min_{\boldsymbol{A}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|_{\mathrm{F}}^2 \\ &= \arg\min_{\boldsymbol{A}} \operatorname{tr}\Big((\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A})^\top (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A})\Big) \\ &= \arg\min_{\boldsymbol{A}} \operatorname{tr}(\boldsymbol{Y}^\top\boldsymbol{Y} - 2\boldsymbol{A}^\top\boldsymbol{X}^\top\boldsymbol{Y} + \boldsymbol{A}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{A}).\end{aligned}$$

By differentiating with respect to $\boldsymbol{A}$ and equating to zero

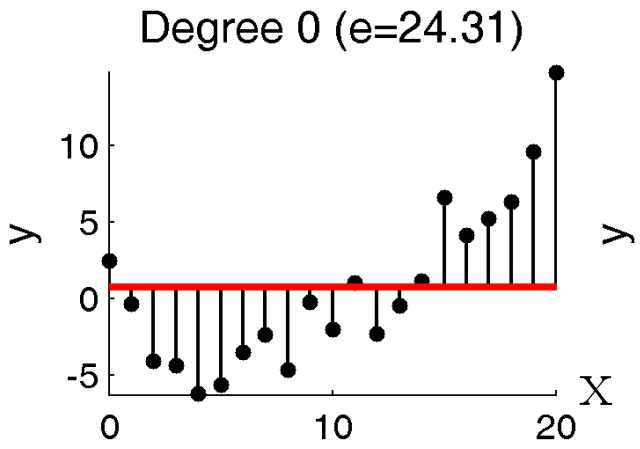
$$-2\boldsymbol{X}^\top\boldsymbol{Y} + 2\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{A} = \boldsymbol{0} \quad \Longleftrightarrow \quad \hat{\boldsymbol{A}} = \boxed{(\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}^\top}\boldsymbol{Y}$$

Moore-Penrose pseudoinverse $\boldsymbol{X}^\dagger$

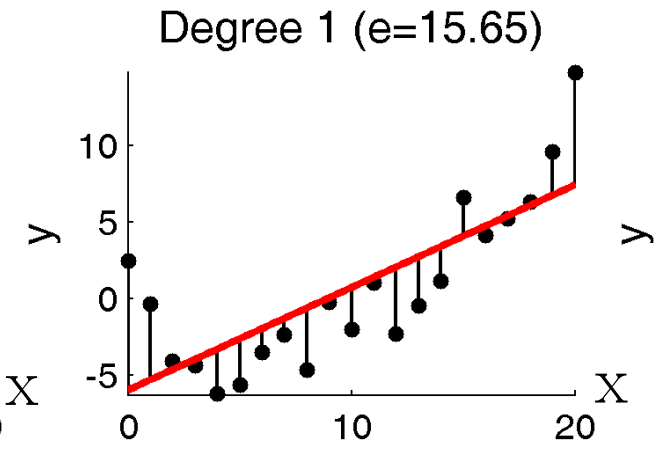


Polynomial fitting with least squares

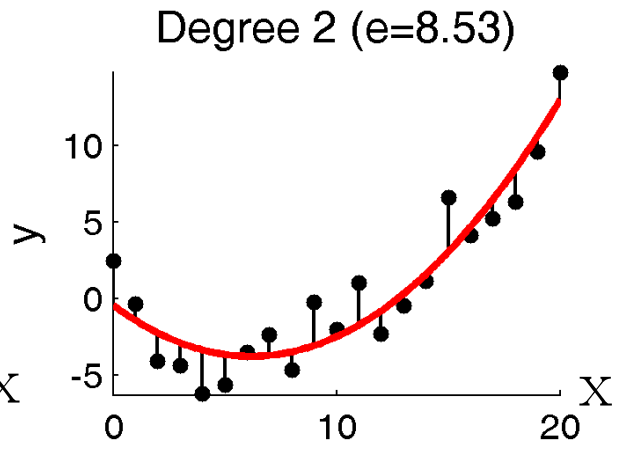
$$\hat{A} = X^{\dagger} Y$$



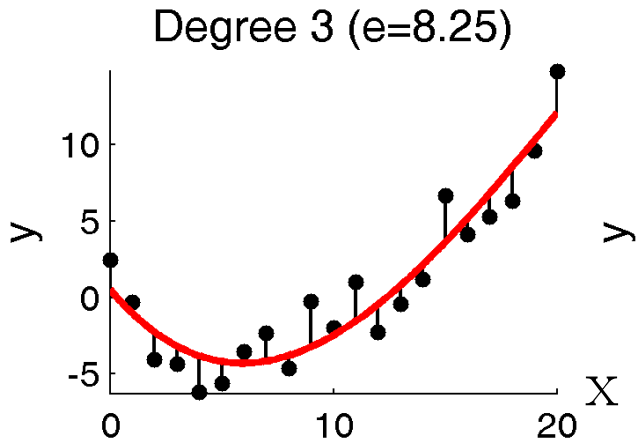
$x = 1$



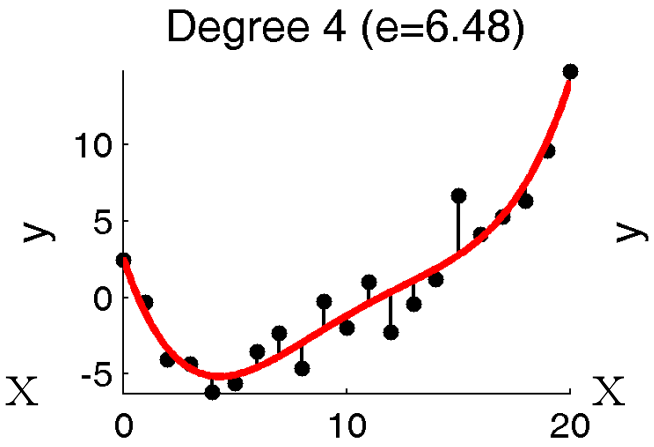
$\boldsymbol{x} = [1, \mathrm{x}]$



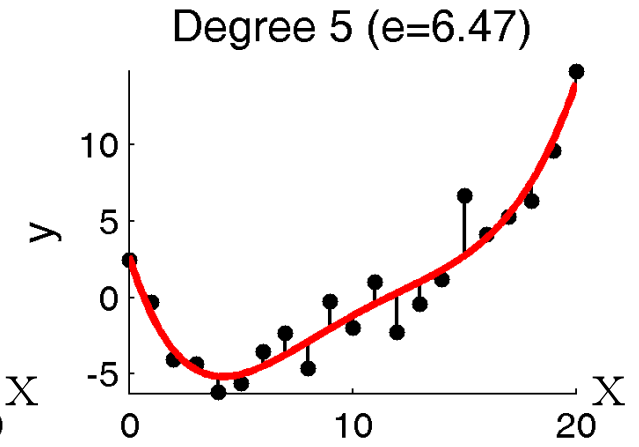
$\boldsymbol{x} = [1, \mathrm{x}, \mathrm{x}^2]$



$\boldsymbol{x} = [1, \mathrm{x}, \mathrm{x}^2, \mathrm{x}^3]$



$\boldsymbol{x} = [1, \mathrm{x}, \mathrm{x}^2, \mathrm{x}^3, \mathrm{x}^4]$



$\boldsymbol{x} = [1, \mathrm{x}, \mathrm{x}^2, \mathrm{x}^3, \mathrm{x}^4, \mathrm{x}^5]$

Least squares computed with SVD

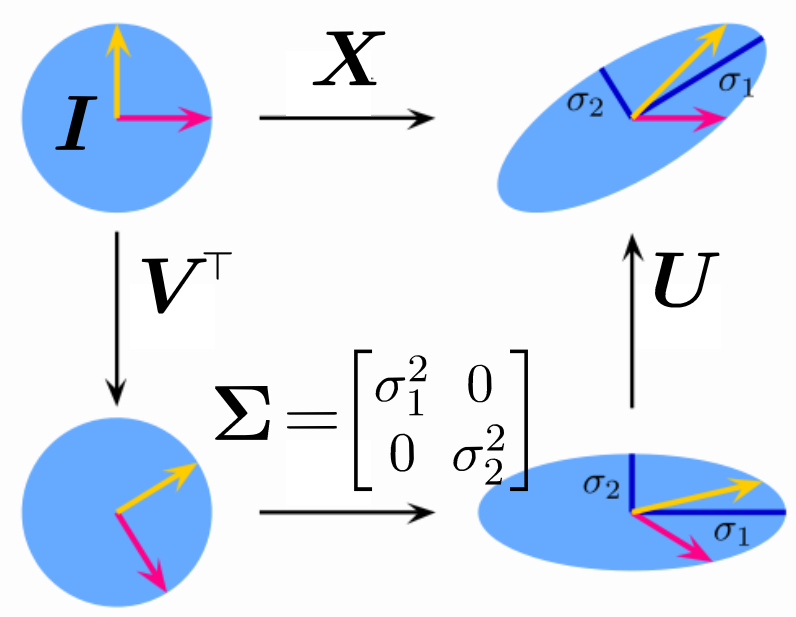
Singular value decomposition (SVD)

$$\overbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \end{bmatrix}}^{\boldsymbol{X} \in \mathbb{R}^{N \times D^{\mathcal{I}}}} = \overbrace{\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \end{bmatrix}}^{\boldsymbol{U} \in \mathbb{R}^{N \times N}} \overbrace{\begin{bmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}}^{\boldsymbol{\Sigma} \in \mathbb{R}^{N \times D^{\mathcal{I}}}} \overbrace{\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \sqrt{0.2} & 0 & 0 & 0 & \sqrt{0.8} \\ 0 & 0 & 0 & 1 & 0 \\ -\sqrt{0.8} & 0 & 0 & 0 & \sqrt{0.2} \end{bmatrix}}^{\boldsymbol{V}^\top \in \mathbb{R}^{D^{\mathcal{I}} \times D^{\mathcal{I}}}}$$

Unitary matrix (orthogonal)

Unitary matrix (orthogonal)

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\top$$



Least squares computed with SVD

$$\boldsymbol{X} \in \mathbb{R}^{N \times D^{\mathcal{I}}}$$

$$\hat{\boldsymbol{A}} = \overbrace{(\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top}^{\boldsymbol{X}^\dagger} \boldsymbol{Y}$$

$\boldsymbol{X}$ can be decomposed with the **singular value decomposition**

$$\boldsymbol{X} = \boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^\top$$

where $\boldsymbol{U}$ and $\boldsymbol{V}$ are $N \times N$ and $D^{\mathcal{I}} \times D^{\mathcal{I}}$ orthogonal matrices, and $\boldsymbol{\Sigma}$ is an $N \times D^{\mathcal{I}}$ matrix with all its elements outside of the main diagonal equal to 0.

$$\boldsymbol{\Sigma} = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0.1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

With this decomposition, a solution to the least squares problem is given by

$$\hat{\boldsymbol{A}} = \boldsymbol{V} \boldsymbol{\Sigma}^\dagger \boldsymbol{U}^\top \boldsymbol{Y}$$

where the pseudoinverse of $\boldsymbol{\Sigma}$ can be easily obtained by inverting the non-zero diagonal elements and transposing the resulting matrix.

$$\boldsymbol{\Sigma}^\dagger = \begin{bmatrix} 0.25 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \\ 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Nullspace projection (kernels in least squares)

Python notebook:
demo_LS_polFit.ipynb

Matlab code:
demo_LS_polFit_nullspace01.m

Nullspace projection

The pseudoinverse provides a single least norm solution, but we can sometimes obtain other solutions by employing a **nullspace projection matrix $\boldsymbol{N}$**

$$\hat{\boldsymbol{A}} = \boldsymbol{X}^{\dagger}\boldsymbol{Y} + \overbrace{(\boldsymbol{I} - \boldsymbol{X}^{\dagger}\boldsymbol{X})}^{\boldsymbol{N}}\boldsymbol{V}.$$

$\boldsymbol{V}$ can be any vector/matrix (typically, a gradient minimizing a secondary objective function).

The nullspace projection guarantees that $\|\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{A}}\|_{\mathrm{F}}^2$ is still minimized.

Nullspace projection computed with SVD

$$\hat{\boldsymbol{A}} = \boldsymbol{X}^{\dagger}\boldsymbol{Y} + \overbrace{(\boldsymbol{I} - \boldsymbol{X}^{\dagger}\boldsymbol{X})}^{\boldsymbol{N}}\boldsymbol{V}$$

An alternative way of computing the nullspace projection matrix is to exploit the singular value decomposition

$$\boldsymbol{X}^{\dagger} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\top}$$

to compute

$$\boldsymbol{N} = \tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^{\top}$$

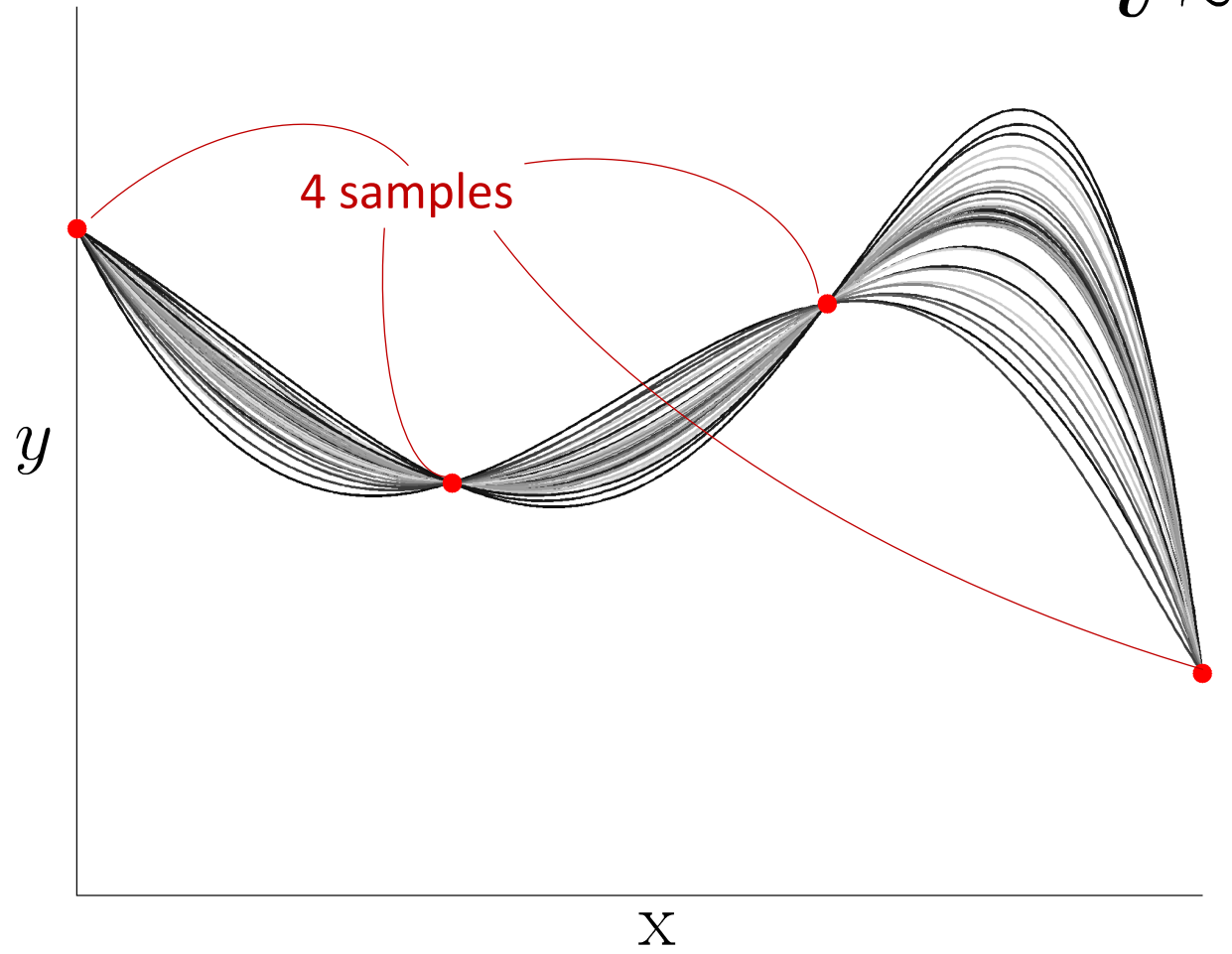
where $\tilde{\boldsymbol{U}}$ is a matrix formed by the columns of $\boldsymbol{U}$ that span for the corresponding zero rows in $\boldsymbol{\Sigma}$.

$$\overbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \end{bmatrix}}^{\boldsymbol{X}^{\dagger} \in \mathbb{R}^{D^{\mathcal{I}} \times N}} = \overbrace{\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \end{bmatrix}}^{\boldsymbol{U} \in \mathbb{R}^{D^{\mathcal{I}} \times D^{\mathcal{I}}}} \overbrace{\begin{bmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}}^{\boldsymbol{\Sigma} \in \mathbb{R}^{D^{\mathcal{I}} \times N}} \overbrace{\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \sqrt{0.2} & 0 & 0 & 0 & \sqrt{0.8} \\ 0 & 0 & 0 & 1 & 0 \\ -\sqrt{0.8} & 0 & 0 & 0 & \sqrt{0.2} \end{bmatrix}}^{\boldsymbol{V}^{\top} \in \mathbb{R}^{N \times N}}$$

$\tilde{\boldsymbol{U}}$

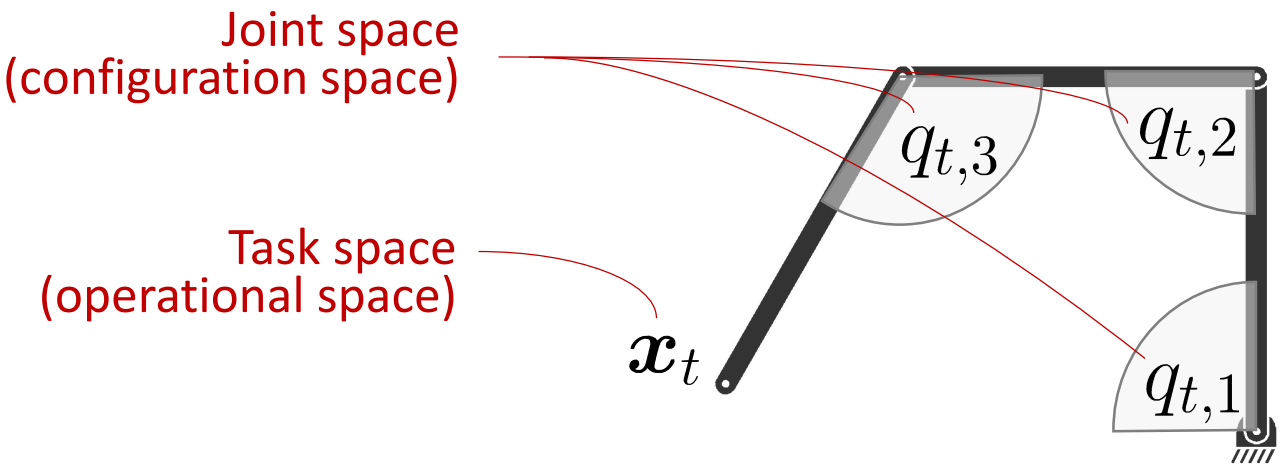
Example: Polynomial fitting

$$\hat{\boldsymbol{a}} = \boldsymbol{X}^{\dagger}\boldsymbol{y} + \boldsymbol{N}\boldsymbol{v} \quad \text{with} \quad \boldsymbol{x} = [1, \mathrm{x}, \mathrm{x}^2, \ldots, \mathrm{x}^6]$$
$$\boldsymbol{v} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$



$$\hat{\boldsymbol{a}} \in \mathbb{R}^7$$
$$\boldsymbol{X} \in \mathbb{R}^{4\times 7}$$
$$\boldsymbol{y} \in \mathbb{R}^4$$
$$\boldsymbol{N} \in \mathbb{R}^{7\times 7}$$
$$\boldsymbol{v} \in \mathbb{R}^7$$

Example: Robot inverse kinematics



Forward kinematics is computed with

$$\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{q}_t) \quad \Longleftrightarrow \quad \dot{\boldsymbol{x}}_t = \frac{\partial \boldsymbol{x}_t}{\partial t} = \frac{\partial \boldsymbol{f}(\boldsymbol{q}_t)}{\partial \boldsymbol{q}_t} \frac{\partial \boldsymbol{q}_t}{\partial t} = \boldsymbol{J}(\boldsymbol{q}_t)\, \dot{\boldsymbol{q}}_t,$$

where $\boldsymbol{J}(\boldsymbol{q}_t) = \frac{\partial \boldsymbol{f}(\boldsymbol{q}_t)}{\partial \boldsymbol{q}_t}$ is a Jacobian matrix.

An inverse kinematics solution can be computed with

$$\hat{\dot{\boldsymbol{q}}}_t = \boldsymbol{J}^{\dagger}(\boldsymbol{q}_t)\, \dot{\boldsymbol{x}}_t + \boldsymbol{N}(\boldsymbol{q}_t)\, \boldsymbol{g}(\boldsymbol{q}_t), \quad \text{where} \quad \boldsymbol{N}(\boldsymbol{q}_t) = \boldsymbol{I} - \boldsymbol{J}^{\dagger}(\boldsymbol{q}_t)\boldsymbol{J}(\boldsymbol{q}_t).$$

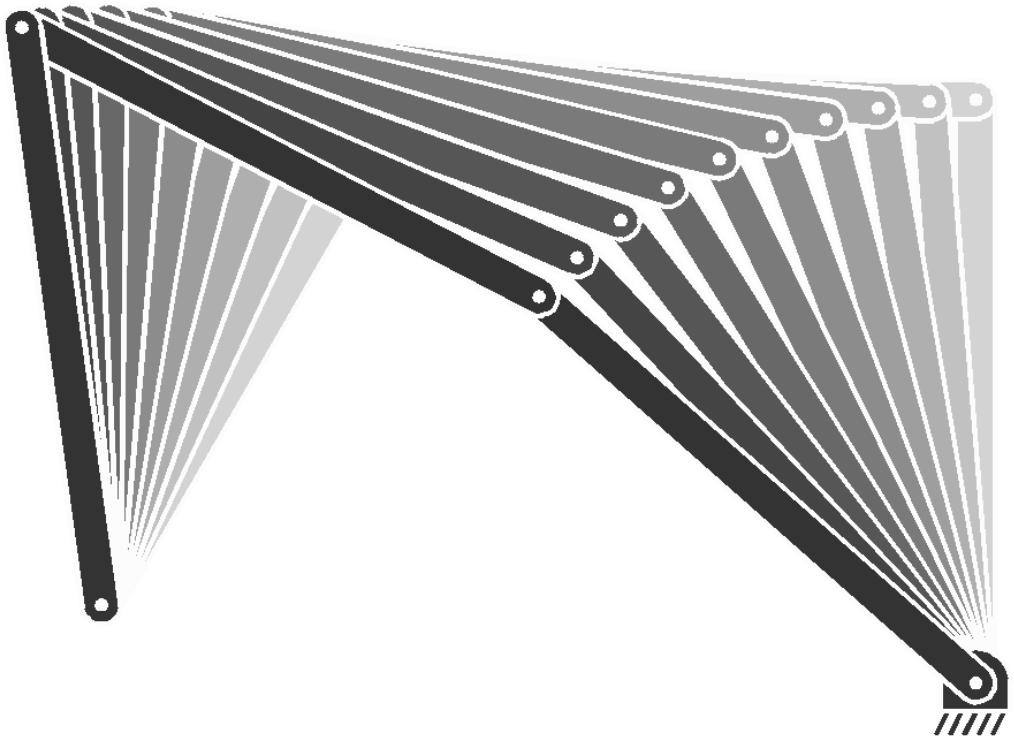
Example: Robot inverse kinematics

Primary constraint:
keeping the tip of
the robot still

$$\hat{\dot{\boldsymbol{q}}}_t = \boldsymbol{J}^{\dagger}(\boldsymbol{q}_t)\ \dot{\boldsymbol{x}}_t \quad + \boldsymbol{N}(\boldsymbol{q}_t)\ \boldsymbol{g}(\boldsymbol{q}_t)$$

$$= \boldsymbol{J}^{\dagger}(\boldsymbol{q}_t) \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad + \boldsymbol{N}(\boldsymbol{q}_t) \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Secondary constraint:
moving the
first joint



Example: Robot inverse kinematics

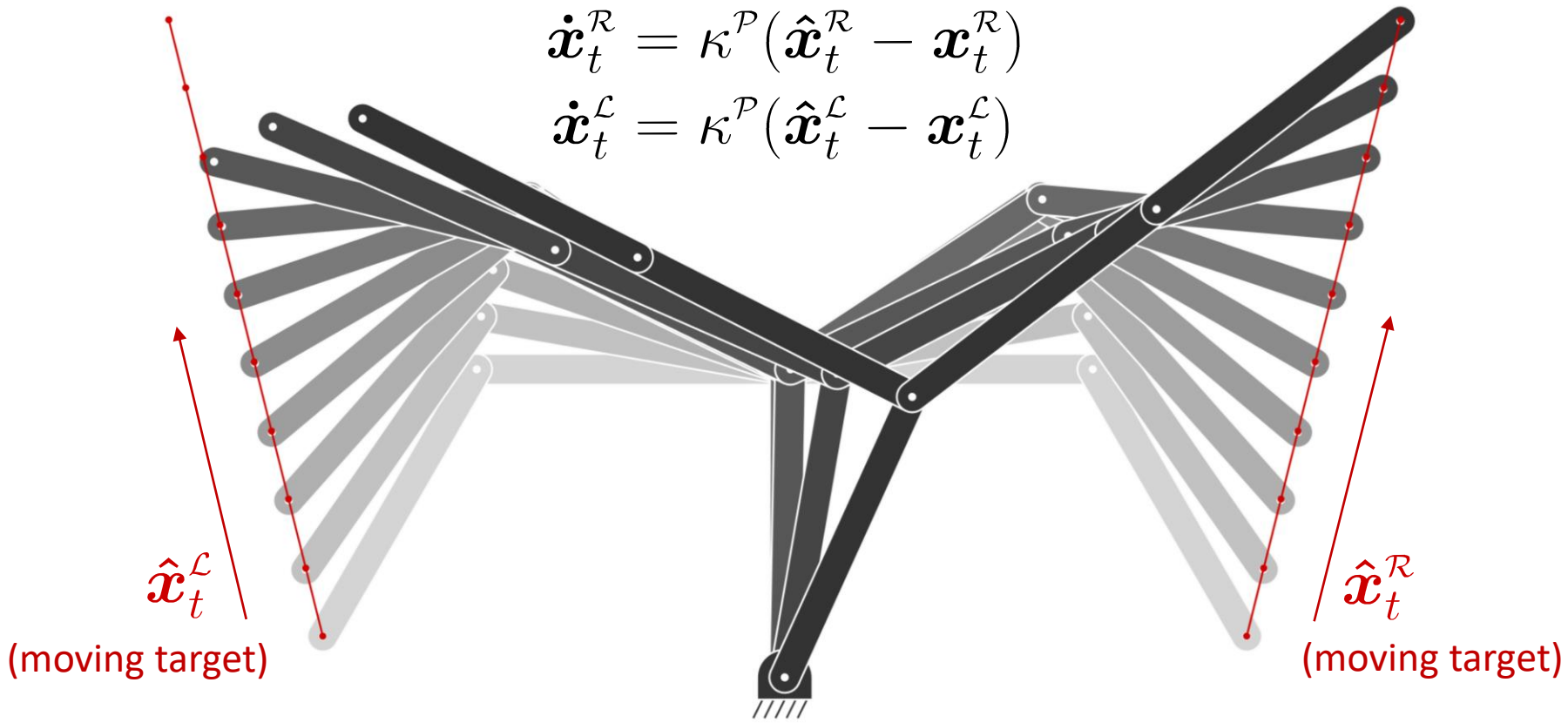
$$\hat{\dot{\boldsymbol{q}}}_t = \boldsymbol{J}_t^{\mathcal{R}\dagger}\, \dot{\boldsymbol{x}}_t^{\mathcal{R}} + \boldsymbol{N}_t^{\mathcal{R}}\, \dot{\boldsymbol{q}}_t^{\mathcal{L}}$$

Tracking target with right hand

Tracking target with left hand, if possible

$$\dot{\boldsymbol{q}}_t^{\mathcal{L}} = (\boldsymbol{J}_t^{\mathcal{L}} \boldsymbol{N}_t^{\mathcal{R}})^{\dagger}\, (\dot{\boldsymbol{x}}_t^{\mathcal{L}} - \boldsymbol{J}_t^{\mathcal{L}}\, \boldsymbol{J}_t^{\mathcal{R}\dagger}\, \dot{\boldsymbol{x}}_t^{\mathcal{R}})$$

$$\dot{\boldsymbol{x}}_t^{\mathcal{R}} = \kappa^{\mathcal{P}}(\hat{\boldsymbol{x}}_t^{\mathcal{R}} - \boldsymbol{x}_t^{\mathcal{R}})$$
$$\dot{\boldsymbol{x}}_t^{\mathcal{L}} = \kappa^{\mathcal{P}}(\hat{\boldsymbol{x}}_t^{\mathcal{L}} - \boldsymbol{x}_t^{\mathcal{L}})$$



Ridge regression

(robust regression, Tikhonov regularization, penalized least squares)

Python notebook:
demo_LS_polFit.ipynb

Matlab example:
demo_LS_polFit02.m

Ridge regression

The least squares objective can be modified to give preference to a particular solution with

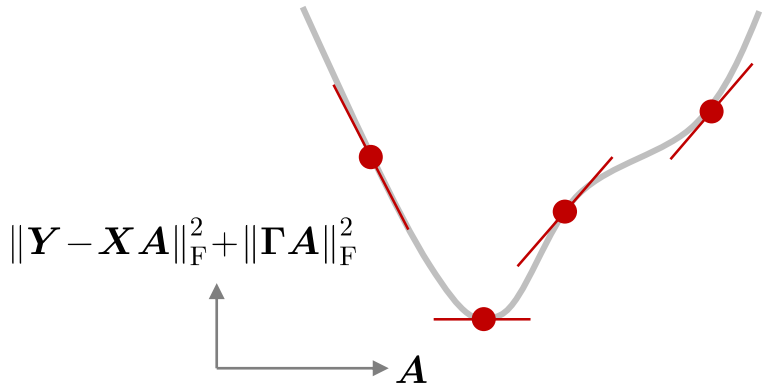
$$\begin{aligned}\hat{\boldsymbol{A}} &= \arg\min_{\boldsymbol{A}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|_{\mathrm{F}}^2 + \|\boldsymbol{\Gamma}\boldsymbol{A}\|_{\mathrm{F}}^2 \\ &= \arg\min_{\boldsymbol{A}} \operatorname{tr}\Big((\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A})^\top(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A})\Big) + \operatorname{tr}\Big((\boldsymbol{\Gamma}\boldsymbol{A})^\top\boldsymbol{\Gamma}\boldsymbol{A}\Big)\end{aligned}$$

By differentiating with respect to $\boldsymbol{A}$ and equating to zero, we can see that

$$-2\boldsymbol{X}^\top\boldsymbol{Y} + 2\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{A} + 2\boldsymbol{\Gamma}^\top\boldsymbol{\Gamma}\boldsymbol{A} = \boldsymbol{0}$$

yielding

$$\hat{\boldsymbol{A}} = (\boldsymbol{X}^\top\boldsymbol{X} + \boldsymbol{\Gamma}^\top\boldsymbol{\Gamma})^{-1}\boldsymbol{X}^\top\boldsymbol{Y}$$



If $\boldsymbol{\Gamma} = \lambda\boldsymbol{I}$ with $0 < \lambda \ll 1$ (i.e., giving preference to solutions with smaller norms), the process is known as **ℓ_2 regularization**.

Ridge regression

Ridge regression can alternatively be computed with augmented matrices

$$\tilde{\boldsymbol{X}} = \begin{bmatrix} \boldsymbol{X} \\ \boldsymbol{\Gamma} \end{bmatrix} \qquad \tilde{\boldsymbol{Y}} = \begin{bmatrix} \boldsymbol{Y} \\ \boldsymbol{0} \end{bmatrix}$$

with $\boldsymbol{0} \in \mathbb{R}^{D^{\mathcal{I}} \times D^{\mathcal{O}}}$ and $\boldsymbol{\Gamma} \in \mathbb{R}^{D^{\mathcal{I}} \times D^{\mathcal{I}}}$, yielding

$$\begin{aligned} \hat{\boldsymbol{A}} &= \left(\tilde{\boldsymbol{X}}^\top \tilde{\boldsymbol{X}}\right)^{-1} \tilde{\boldsymbol{X}}^\top \tilde{\boldsymbol{Y}} \\ &= \left(\begin{bmatrix} \boldsymbol{X} \\ \boldsymbol{\Gamma} \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{X} \\ \boldsymbol{\Gamma} \end{bmatrix}\right)^{-1} \begin{bmatrix} \boldsymbol{X} \\ \boldsymbol{\Gamma} \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{Y} \\ \boldsymbol{0} \end{bmatrix} \\ &= \left(\boldsymbol{X}^\top \boldsymbol{X} + \boldsymbol{\Gamma}^\top \boldsymbol{\Gamma}\right)^{-1} \boldsymbol{X}^\top \boldsymbol{Y} \end{aligned}$$

$$\begin{aligned} \boldsymbol{X} &\in \mathbb{R}^{N \times D^{\mathcal{I}}} \\ \boldsymbol{Y} &\in \mathbb{R}^{N \times D^{\mathcal{O}}} \\ \boldsymbol{A} &\in \mathbb{R}^{D^{\mathcal{I}} \times D^{\mathcal{O}}} \end{aligned}$$

Ridge regression computed with SVD

For the singular value decomposition

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\top$$

with σ_i the singular values in the diagonal of $\boldsymbol{\Sigma}$, a solution to the ridge regression problem is given by

$$\hat{\boldsymbol{A}} = \boldsymbol{V}\tilde{\boldsymbol{\Sigma}}\boldsymbol{U}^\top \boldsymbol{Y}$$

where $\tilde{\boldsymbol{\Sigma}}$ has diagonal values

$$\tilde{\sigma}_i = \frac{\sigma_i}{\sigma_i^2 + \lambda}$$

and has zeros elsewhere.

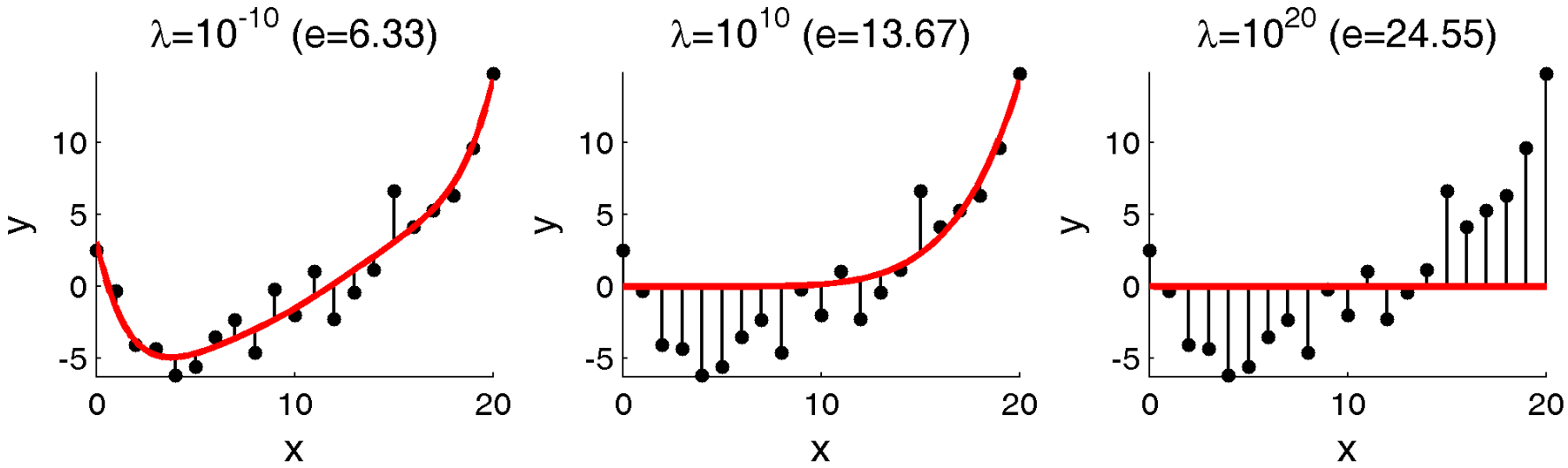
$$\boldsymbol{\Sigma} = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0.1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\tilde{\boldsymbol{\Sigma}} = \begin{bmatrix} 0.2498 & 0 & 0 & 0 \\ 0 & 0.4988 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

(for $\lambda = 0.01$)

Example: Polynomial fitting

$D^{\mathcal{I}} = 7$ (polynomial of degree 6)



Weighted least squares
(Generalized least squares)

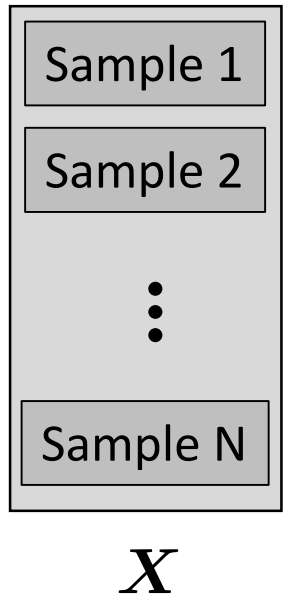
Python notebook:
demo_LS_weighted.ipynb

Matlab example:
demo_LS_weighted01.m

Weighted least squares

By describing the input data as $\boldsymbol{X} \in \mathbb{R}^{N \times D^{\mathcal{I}}}$ and the output data as $\boldsymbol{Y} \in \mathbb{R}^{N \times D^{\mathcal{O}}}$, with a weight matrix $\boldsymbol{W} \in \mathbb{R}^{N \times N}$, we want to minimize

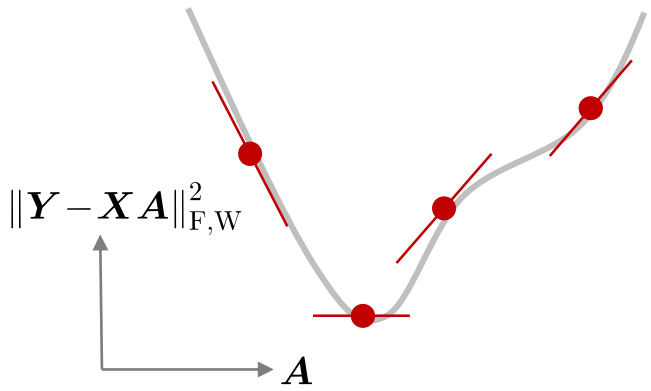
$$\begin{aligned}\hat{\boldsymbol{A}} &= \arg\min_{\boldsymbol{A}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|^2_{\mathrm{F},\boldsymbol{W}} \\ &= \arg\min_{\boldsymbol{A}} \operatorname{tr}\Big((\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A})^\top \boldsymbol{W}(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A})\Big) \\ &= \arg\min_{\boldsymbol{A}} \operatorname{tr}(\boldsymbol{Y}^\top\boldsymbol{W}\boldsymbol{Y} - 2\boldsymbol{A}^\top\boldsymbol{X}^\top\boldsymbol{W}\boldsymbol{Y} + \boldsymbol{A}^\top\boldsymbol{X}^\top\boldsymbol{W}\boldsymbol{X}\boldsymbol{A}).\end{aligned}$$



By differentiating with respect to $\boldsymbol{A}$ and equating to zero

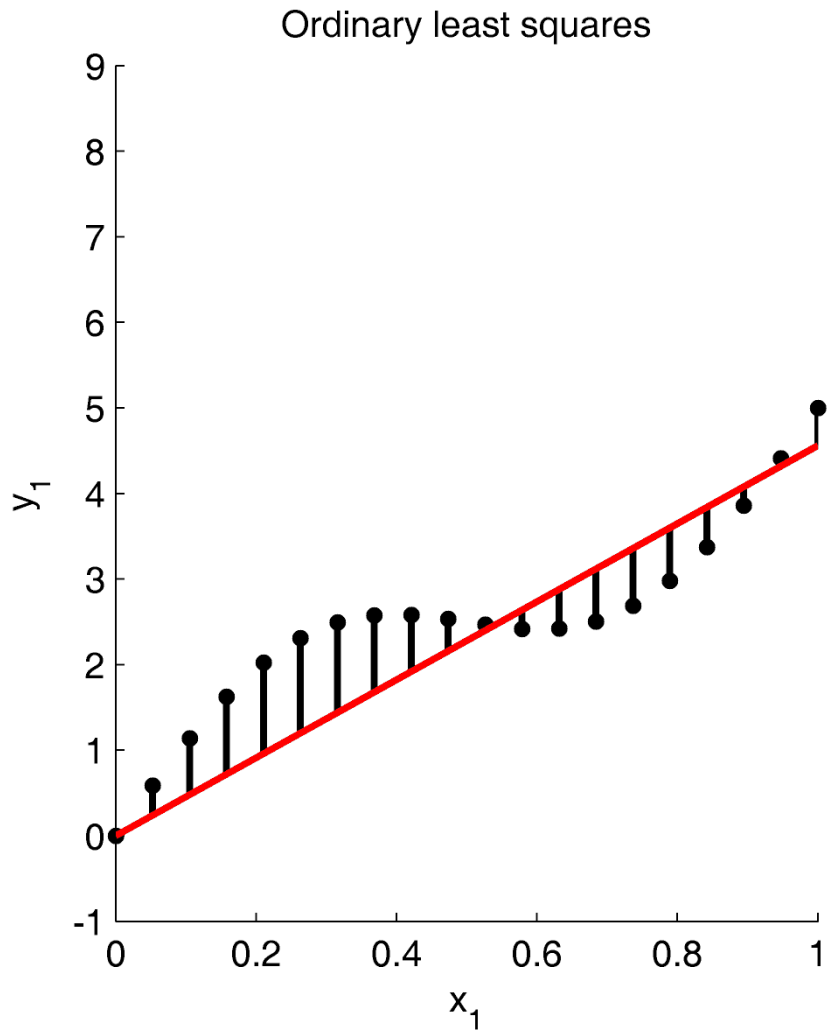
$$-2\boldsymbol{X}^\top\boldsymbol{W}\boldsymbol{Y} + 2\boldsymbol{X}^\top\boldsymbol{W}\boldsymbol{X}\boldsymbol{A} = \boldsymbol{0} \iff \hat{\boldsymbol{A}} = \boxed{(\boldsymbol{X}^\top\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}^\top\boldsymbol{W}}\boldsymbol{Y}$$

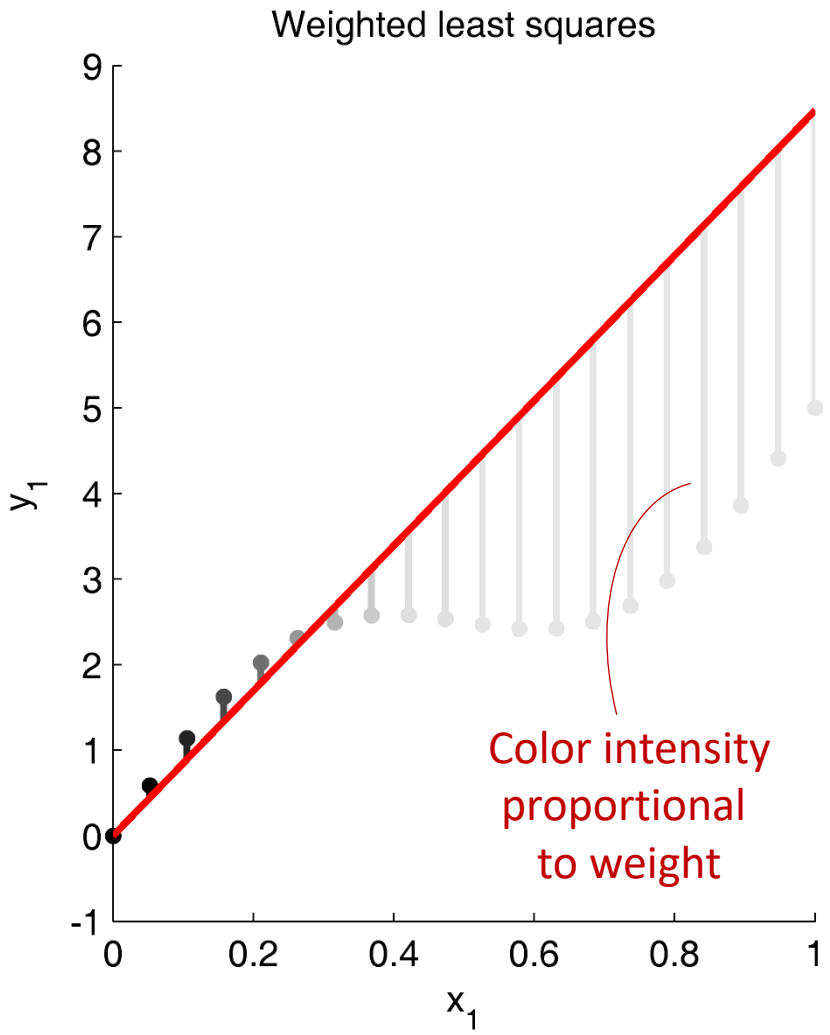
$$\boldsymbol{X}^\dagger_{\boldsymbol{W}}$$



Weighted least squares

$$\hat{A} = (X^\top W X)^{-1} X^\top W Y$$

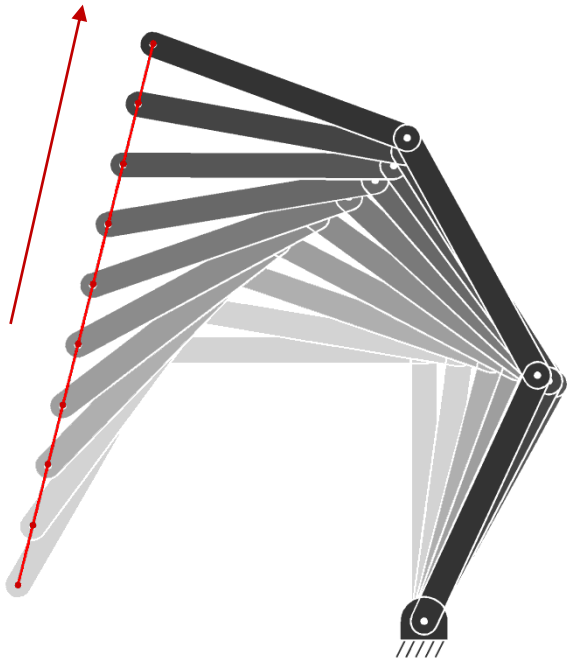


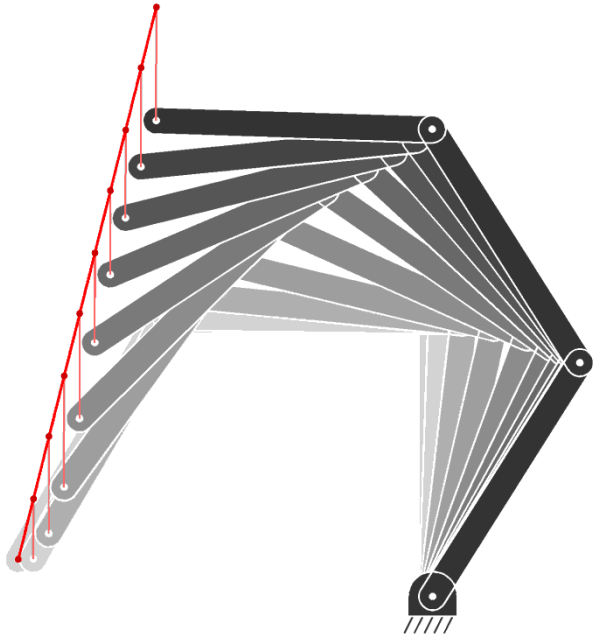


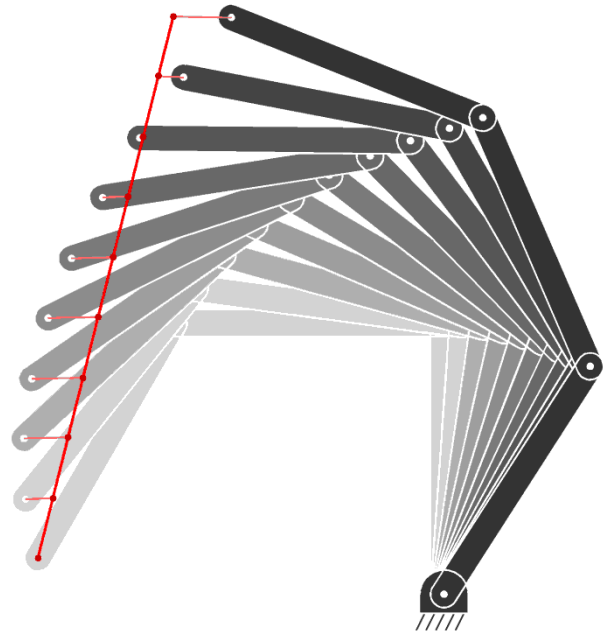
Example: Robot inverse kinematics (weights in task space)

$$\hat{\dot{\boldsymbol{q}}}_t = (\boldsymbol{J}^\top \boldsymbol{W}^x \boldsymbol{J} + \lambda \boldsymbol{I}_{\boldsymbol{q}})^{-1} \boldsymbol{J}^\top \boldsymbol{W}^x \, \dot{\boldsymbol{x}}_t$$

(moving target)







$$\boldsymbol{W}^x = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

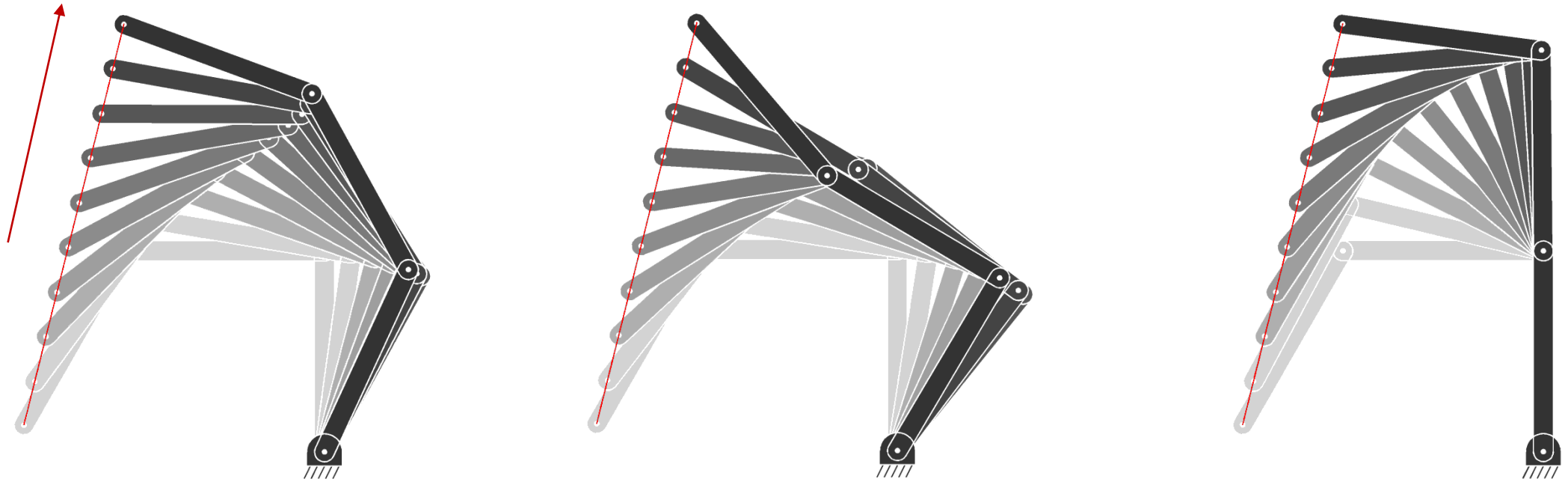
$$\boldsymbol{W}^x = \begin{bmatrix} 1 & 0 \\ 0 & .01 \end{bmatrix}$$

$$\boldsymbol{W}^x = \begin{bmatrix} .01 & 0 \\ 0 & 1 \end{bmatrix}$$

Example: Robot inverse kinematics (weights in joint space)

$$\hat{\dot{\boldsymbol{q}}}_t = \boldsymbol{W}^{\mathcal{Q}} \boldsymbol{J}^\top (\boldsymbol{J} \boldsymbol{W}^{\mathcal{Q}} \boldsymbol{J}^\top + \lambda \boldsymbol{I}_{\boldsymbol{x}})^{-1} \dot{\boldsymbol{x}}_t$$

(moving target)



$$\boldsymbol{W}^{\mathcal{Q}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\boldsymbol{W}^{\mathcal{Q}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & .01 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\boldsymbol{W}^{\mathcal{Q}} = \begin{bmatrix} .01 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Iteratively reweighted least squares (IRLS)

Python notebook:
demo_LS_weighted.ipynb

Matlab code:
demo_LS_IRLS01.m

Iteratively reweighted least squares (IRLS)

- **Iteratively Reweighted Least Squares (IRLS)** generalizes least squares by raising the error term to a power that is less than 2:
  → the optimization problem can no longer be called “least squares”

- The strategy of IRLS is that an error $|\mathbf{e}|^p$ can be rewritten as $|\mathbf{e}|^p = |\mathbf{e}|^{p-2}\,\mathbf{e}^2$.

- $|\mathbf{e}|^{p-2}$ can be interpreted as a weight, which is used to minimize $\mathbf{e}^2$ with **weighted least squares**.
  → we solve a least squares problem at each iteration of the algorithm

- p=1 corresponds to **least absolute deviation regression**.

Iteratively reweighted least squares (IRLS)

$|e|^p = |e|^{p-2} e^2$

transformed as weight **W**

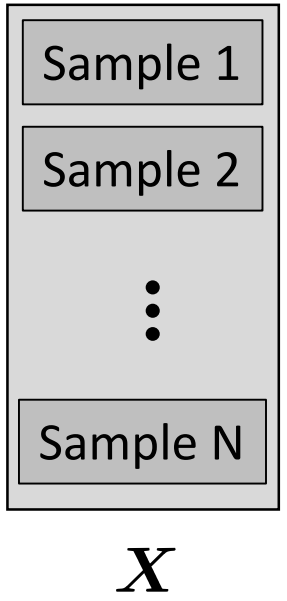
For an ℓ_p norm cost function defined by

$$\hat{\boldsymbol{A}} = \arg\min_{\boldsymbol{A}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|_{\mathrm{F},p}^2$$

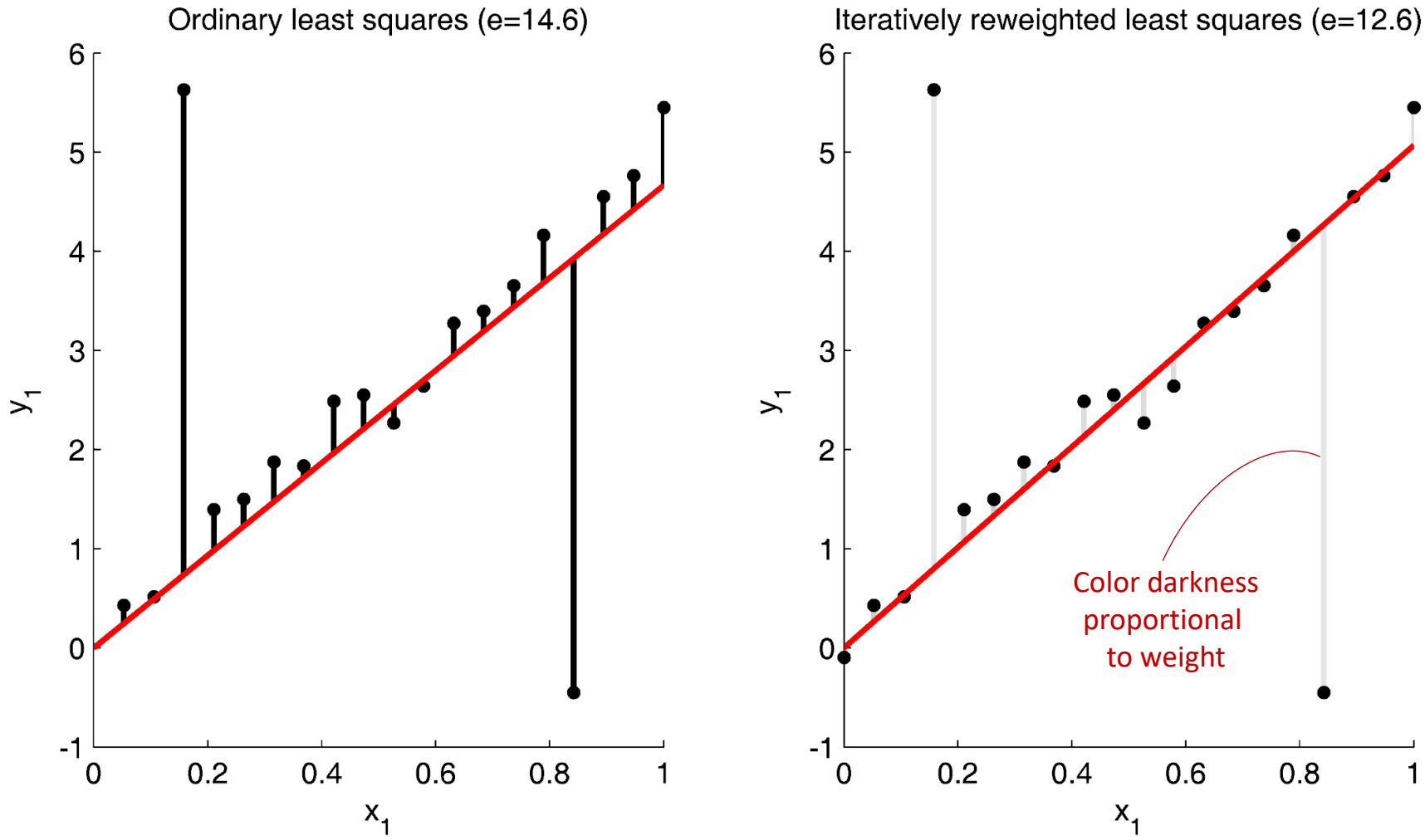
$\hat{\boldsymbol{A}}$ is estimated by starting from $\boldsymbol{W} = \boldsymbol{I}$ and iteratively computing

$$\hat{\boldsymbol{A}} \leftarrow (\boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{Y}$$

$$\boldsymbol{W}_{n,n} \leftarrow |\boldsymbol{Y}_n - \boldsymbol{X}_n \boldsymbol{A}|^{p-2} \quad \forall n \in \{1, \ldots, N\}$$



Iteratively reweighted least squares (IRLS)



→ regression that can be more robust to outliers

Recursive least squares

Python notebook:
demo_LS_recursive.ipynb

Matlab code:
demo_LS_recursive01.m

Recursive least squares

Sherman-Morrison-Woodbury relation:

$$(\boldsymbol{B}+\boldsymbol{U}\boldsymbol{V})^{-1} = \boldsymbol{B}^{-1} - \overbrace{\boldsymbol{B}^{-1}\boldsymbol{U}\left(\boldsymbol{I}+\boldsymbol{V}\boldsymbol{B}^{-1}\boldsymbol{U}\right)^{-1}\boldsymbol{V}\boldsymbol{B}^{-1}}^{\boldsymbol{E}}$$

with $\boldsymbol{U}\in\mathbb{R}^{n\times m}$ and $\boldsymbol{V}\in\mathbb{R}^{m\times n}$.

When $m \ll n$, the correction term $\boldsymbol{E}$ can be computed more efficiently than inverting $\boldsymbol{B}+\boldsymbol{U}\boldsymbol{V}$.

By defining $\boldsymbol{B}=\boldsymbol{X}^\top\boldsymbol{X}$, the above relation can be exploited to update a least squares solution when new datapoints are available.

$$\hat{\boldsymbol{A}} = \overbrace{\left(\boldsymbol{X}^\top\boldsymbol{X}\right)^{-1}\boldsymbol{X}^\top}^{\boldsymbol{X}^\dagger}\boldsymbol{Y}$$

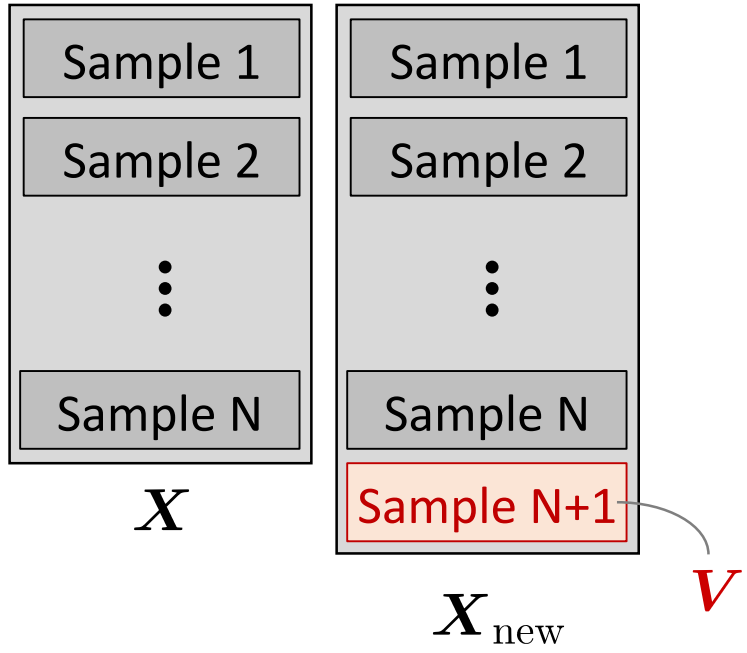
$$\boldsymbol{X}\in\mathbb{R}^{N\times D^{\mathcal{I}}}$$

$$\boldsymbol{X}_{\text{new}}\in\mathbb{R}^{N_{\text{new}}\times D^{\mathcal{I}}}$$

Recursive least squares

If $\boldsymbol{X}_{\text{new}} = [\boldsymbol{X}^\top, \boldsymbol{V}^\top]^\top$ and $\boldsymbol{Y}_{\text{new}} = [\boldsymbol{Y}^\top, \boldsymbol{C}^\top]^\top$, we then have

$$\begin{aligned}\boldsymbol{B}_{\text{new}} &= \boldsymbol{X}_{\text{new}}^\top \boldsymbol{X}_{\text{new}} \\ &= \boldsymbol{X}^\top \boldsymbol{X} + \boldsymbol{V}^\top \boldsymbol{V} \\ &= \boldsymbol{B} + \boldsymbol{V}^\top \boldsymbol{V}\end{aligned}$$



whose inverse can be computed with

$$\boldsymbol{B}_{\text{new}}^{-1} = \boldsymbol{B}^{-1} - \boldsymbol{B}^{-1}\boldsymbol{V}^\top \left(\boldsymbol{I} + \boldsymbol{V}\boldsymbol{B}^{-1}\boldsymbol{V}^\top\right)^{-1} \boldsymbol{V}\boldsymbol{B}^{-1}$$

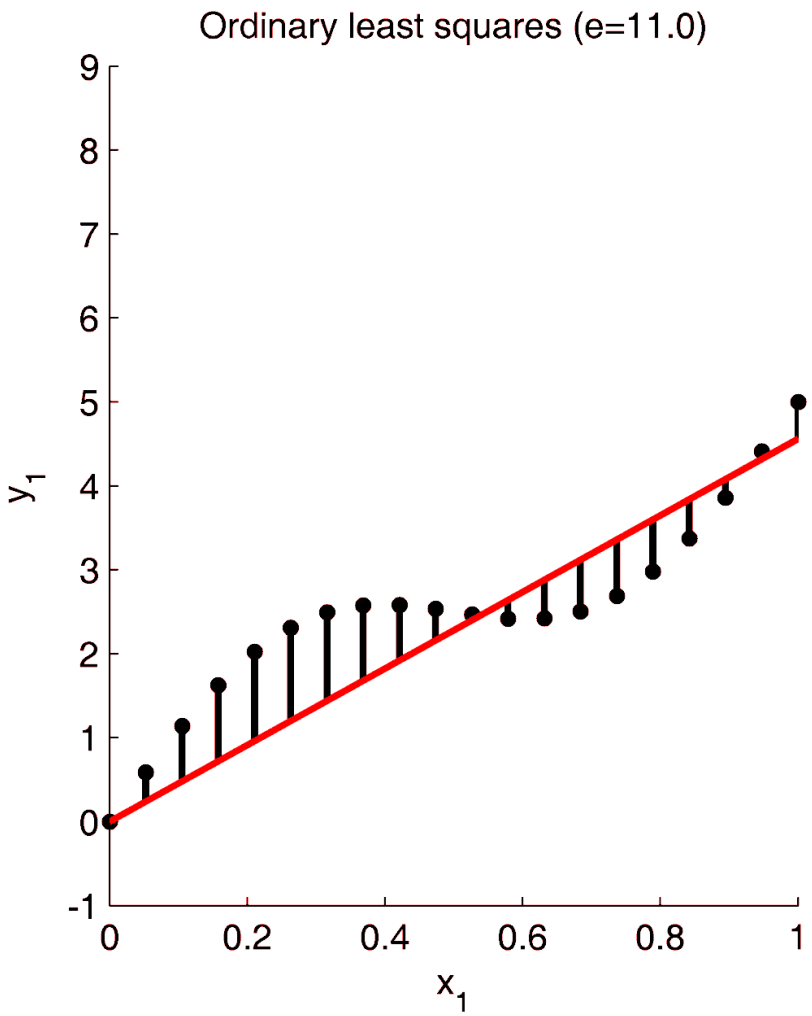
which is exploited to efficiently compute the lease squares update as

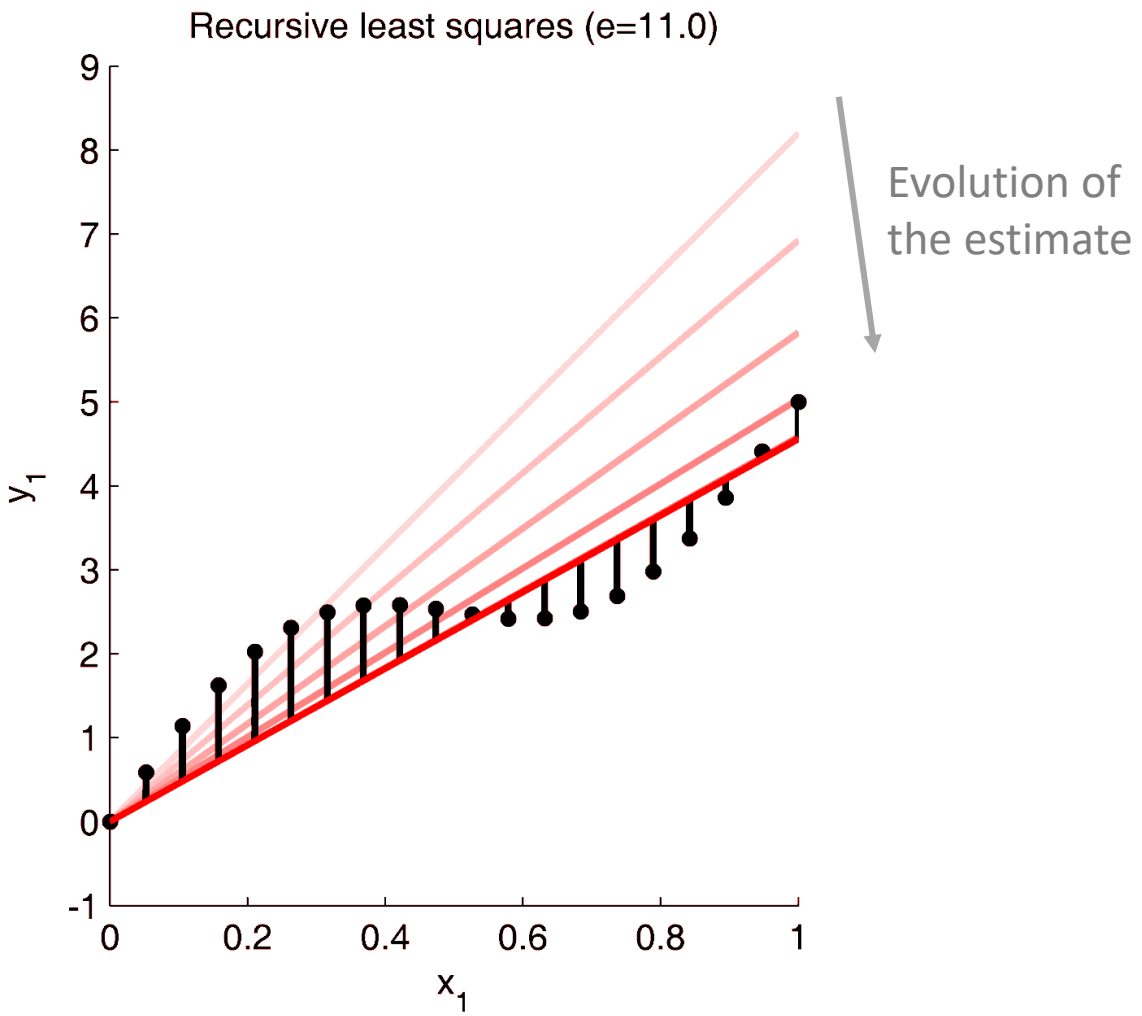
$$\hat{\boldsymbol{A}}_{\text{new}} = \hat{\boldsymbol{A}} + \boldsymbol{K}\left(\boldsymbol{C} - \boldsymbol{V}\hat{\boldsymbol{A}}\right)$$

with Kalman gain $\boldsymbol{K} = \boldsymbol{B}^{-1}\boldsymbol{V}^\top \left(\boldsymbol{I} + \boldsymbol{V}\boldsymbol{B}^{-1}\boldsymbol{V}^\top\right)^{-1}$

$$(\boldsymbol{B} + \boldsymbol{U}\boldsymbol{V})^{-1} = \boldsymbol{B}^{-1} - \overbrace{\boldsymbol{B}^{-1}\boldsymbol{U}\left(\boldsymbol{I} + \boldsymbol{V}\boldsymbol{B}^{-1}\boldsymbol{U}\right)^{-1}\boldsymbol{V}\boldsymbol{B}^{-1}}^{\boldsymbol{E}}$$

Recursive least squares





→ the least squares estimate is the same in the two cases

Linear regression:

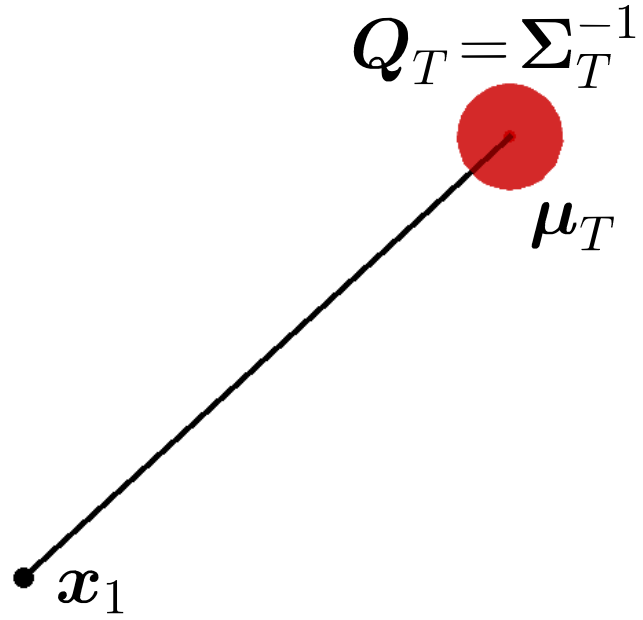
Example of application

Linear quadratic tracking (LQT)

Track path! Use low control commands!

$$\min_{\boldsymbol{u}} \sum_{t=1}^{T} \|\boldsymbol{\mu}_t - \boldsymbol{x}_t\|^2_{\boldsymbol{Q}_t} + \|\boldsymbol{u}_t\|^2_{\boldsymbol{R}_t}$$

$$\text{s.t. } \boldsymbol{x}_{t+1} = \boldsymbol{A}\boldsymbol{x}_t + \boldsymbol{B}\boldsymbol{u}_t$$ System dynamics



$\boldsymbol{x}_t$ state variable (position+velocity)

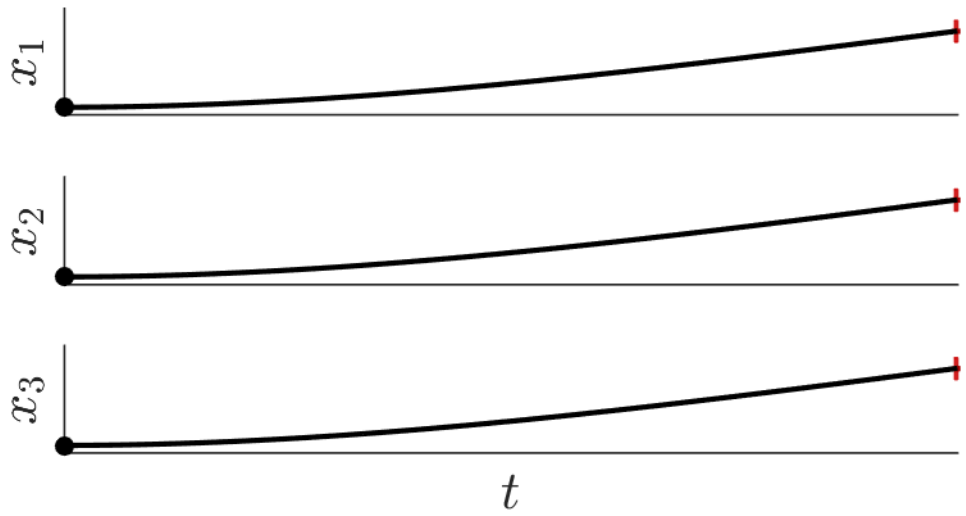
$\boldsymbol{\mu}_t$ desired state

$\boldsymbol{u}_t$ control command (acceleration)

$\boldsymbol{Q}_t$ precision matrix

$\boldsymbol{R}_t$ control weight matrix

$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{u}_2 \\ \vdots \\ \boldsymbol{u}_T \end{bmatrix}$$



Linear quadratic tracking (LQT)

Track path! Use low control commands!

$$\min_{\boldsymbol{u}} \sum_{t=1}^{T} \|\boldsymbol{\mu}_t - \boldsymbol{x}_t\|^2_{\boldsymbol{Q}_t} + \|\boldsymbol{u}_t\|^2_{\boldsymbol{R}_t}$$

$$\text{s.t. } \boldsymbol{x}_{t+1} = \boldsymbol{A}\boldsymbol{x}_t + \boldsymbol{B}\boldsymbol{u}_t$$

System dynamics

Pontryagin's max. principle, Riccati equation, Hamilton-Jacobi-Bellman

(the Physicist perspective)

Dynamic programming

(the Computer Scientist perspective)

Linear algebra

(the Algebraist perspective)

Linear quadratic tracking (LQT)

$$
\begin{aligned}
c &= \sum_{t=1}^{T} \Big((\boldsymbol{\mu}_t - \boldsymbol{x}_t)^\top \boldsymbol{Q}_t (\boldsymbol{\mu}_t - \boldsymbol{x}_t) \;+\; \boldsymbol{u}_t^\top \boldsymbol{R}_t \boldsymbol{u}_t \Big) \\
&= (\boldsymbol{\mu} - \boldsymbol{x})^\top \boldsymbol{Q} (\boldsymbol{\mu} - \boldsymbol{x}) \;+\; \boldsymbol{u}^\top \boldsymbol{R} \boldsymbol{u}
\end{aligned}
$$

$$
\boldsymbol{u} = \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{u}_2 \\ \vdots \\ \boldsymbol{u}_T \end{bmatrix}
$$

$$
\boldsymbol{Q} = \begin{bmatrix} \boldsymbol{Q}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{Q}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{Q}_T \end{bmatrix}
$$

$$
\boldsymbol{R} = \begin{bmatrix} \boldsymbol{R}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{R}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{R}_T \end{bmatrix}
$$

$$
\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \\ \vdots \\ \boldsymbol{\mu}_T \end{bmatrix}
\qquad
\boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \vdots \\ \boldsymbol{x}_T \end{bmatrix}
$$

Linear quadratic tracking (LQT)

$$\boldsymbol{x}_{t+1} = \boldsymbol{A}\,\boldsymbol{x}_t + \boldsymbol{B}\,\boldsymbol{u}_t$$

$$\begin{aligned}
\boldsymbol{x}_2 &= \boldsymbol{A}\boldsymbol{x}_1 + \boldsymbol{B}\boldsymbol{u}_1 \\
\boldsymbol{x}_3 &= \boldsymbol{A}\boldsymbol{x}_2 + \boldsymbol{B}\boldsymbol{u}_2 = \boldsymbol{A}(\boldsymbol{A}\boldsymbol{x}_1 + \boldsymbol{B}\boldsymbol{u}_1) + \boldsymbol{B}\boldsymbol{u}_2 \\
&\vdots \\
\boldsymbol{x}_T &= \boldsymbol{A}^{T-1}\boldsymbol{x}_1 + \boldsymbol{A}^{T-2}\boldsymbol{B}\boldsymbol{u}_1 + \boldsymbol{A}^{T-3}\boldsymbol{B}\boldsymbol{u}_2 + \cdots + \boldsymbol{B}_{T-1}\boldsymbol{u}_{T-1}
\end{aligned}$$

$$\begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{x}_3 \\ \vdots \\ \boldsymbol{x}_T \end{bmatrix} = \underbrace{\begin{bmatrix} \boldsymbol{I} \\ \boldsymbol{A} \\ \boldsymbol{A}^2 \\ \vdots \\ \boldsymbol{A}^{T-1} \end{bmatrix}}_{\boldsymbol{S}^{\boldsymbol{x}}} \boldsymbol{x}_1 + \underbrace{\begin{bmatrix} \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{B} & \boldsymbol{0} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{A}\boldsymbol{B} & \boldsymbol{B} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \boldsymbol{A}^{T-2}\boldsymbol{B} & \boldsymbol{A}^{T-3}\boldsymbol{B} & \cdots & \boldsymbol{B} & \boldsymbol{0} \end{bmatrix}}_{\boldsymbol{S}^{\boldsymbol{u}}} \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{u}_2 \\ \vdots \\ \boldsymbol{u}_T \end{bmatrix}$$

$$\boldsymbol{x} = \boldsymbol{S}^{\boldsymbol{x}}\boldsymbol{x}_1 + \boldsymbol{S}^{\boldsymbol{u}}\boldsymbol{u}$$

Linear quadratic tracking (LQT)

The constraint can then be inserted in the cost function:

$$x = S^x x_1 + S^u u$$

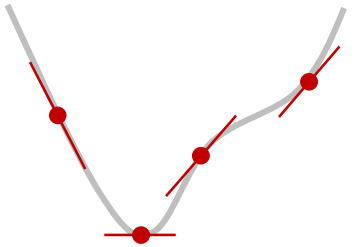
$$c = (\mu - x)^\top Q(\mu - x) + u^\top R u$$

$$= (\mu - S^x x_1 - S^u u)^\top Q (\mu - S^x x_1 - S^u u) + u^\top R u$$

Solving for *u* is similar to a weighted ridge regression problem, and results in the analytic solution:

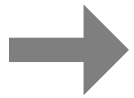
$$\hat{u} = (S^{u\top} Q S^u + R)^{-1} S^{u\top} Q (\mu - S^x x_1)$$

$$\hat{u} = \begin{bmatrix} \hat{u}_1 \\ \hat{u}_2 \\ \vdots \\ \hat{u}_T \end{bmatrix}$$



Linear quadratic tracking (LQT)

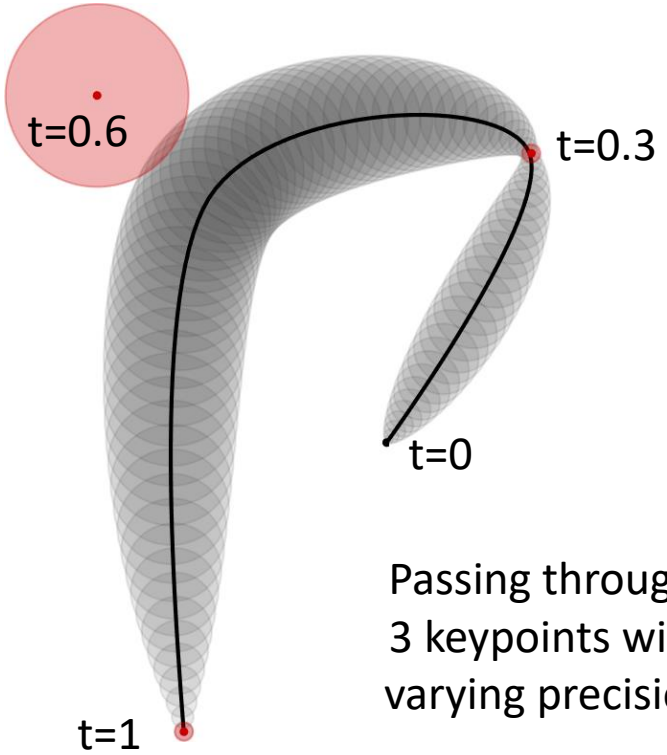
$$\hat{\boldsymbol{u}} = \left(\boldsymbol{S}^{\boldsymbol{u}\top}\boldsymbol{Q}\boldsymbol{S}^{\boldsymbol{u}} + \boldsymbol{R}\right)^{-1}\boldsymbol{S}^{\boldsymbol{u}\top}\boldsymbol{Q}\left(\boldsymbol{\mu} - \boldsymbol{S}^{\boldsymbol{x}}\boldsymbol{x}_1\right)$$
$$\hat{\boldsymbol{\Sigma}}^{\boldsymbol{u}} = \left(\boldsymbol{S}^{\boldsymbol{u}\top}\boldsymbol{Q}\boldsymbol{S}^{\boldsymbol{u}} + \boldsymbol{R}\right)^{-1}$$



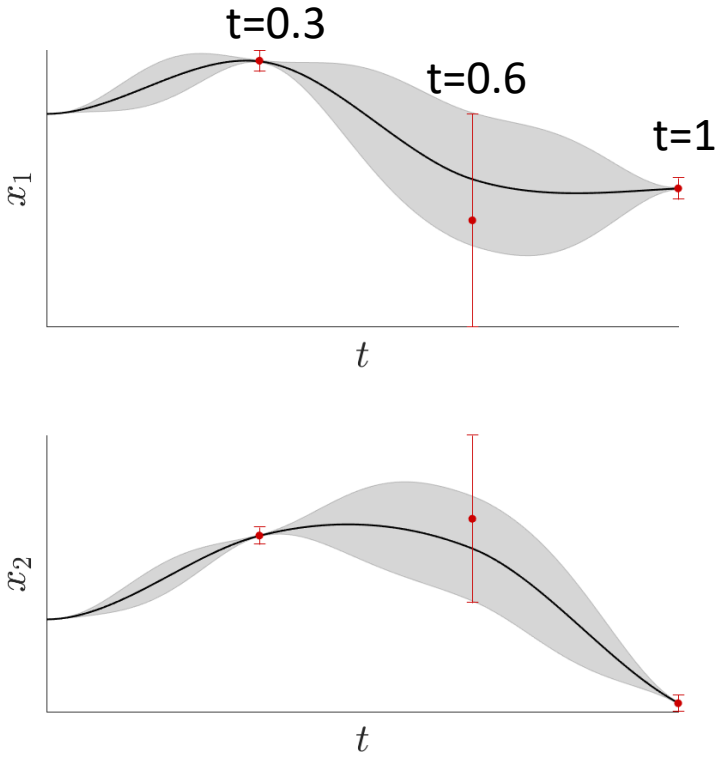
$$\hat{\boldsymbol{x}} = \boldsymbol{S}^{\boldsymbol{x}}\boldsymbol{x}_1 + \boldsymbol{S}^{\boldsymbol{u}}\hat{\boldsymbol{u}}$$
$$\hat{\boldsymbol{\Sigma}}^{\boldsymbol{x}} = \boldsymbol{S}^{\boldsymbol{u}}\left(\boldsymbol{S}^{\boldsymbol{u}\top}\boldsymbol{Q}\boldsymbol{S}^{\boldsymbol{u}} + \boldsymbol{R}\right)^{-1}\boldsymbol{S}^{\boldsymbol{u}\top}$$

The error on the regression estimate can be used to form a distribution

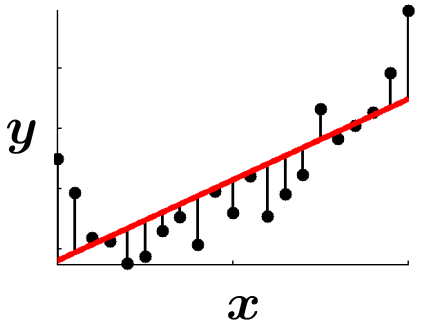
The distribution in control space can then be projected back to the state space



Passing through
3 keypoints with
varying precision



Linear quadratic tracking (LQT) - Example



For $t \leq \frac{T}{4}$ (left hand holding the ball), we have

$$\underbrace{\begin{bmatrix} \dot{\mathbf{x}}_{1,t} \\ \ddot{\mathbf{x}}_{1,t} \\ \dot{\boldsymbol{f}}_{1,t} \\ \hline \dot{\mathbf{x}}_{2,t} \\ \ddot{\mathbf{x}}_{2,t} \\ \dot{\boldsymbol{f}}_{2,t} \\ \hline \dot{\mathbf{x}}_{3,t} \\ \ddot{\mathbf{x}}_{3,t} \\ \dot{\boldsymbol{f}}_{3,t} \end{bmatrix}}_{\dot{\boldsymbol{x}}_t} = \underbrace{\left[\begin{array}{ccccccccc} \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{array}\right]}_{\boldsymbol{A}_t^c} \underbrace{\begin{bmatrix} \mathbf{x}_{1,t} \\ \dot{\mathbf{x}}_{1,t} \\ \boldsymbol{f}_{1,t} \\ \hline \mathbf{x}_{2,t} \\ \dot{\mathbf{x}}_{2,t} \\ \boldsymbol{f}_{2,t} \\ \hline \mathbf{x}_{3,t} \\ \dot{\mathbf{x}}_{3,t} \\ \boldsymbol{f}_{3,t} \end{bmatrix}}_{\boldsymbol{x}_t} + \underbrace{\left[\begin{array}{cc} \mathbf{0} & \mathbf{0} \\ \boldsymbol{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I} \\ \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{array}\right]}_{\boldsymbol{B}_t^c} \underbrace{\left[\begin{array}{c} \boldsymbol{u}_{1,t} \\ \hline \boldsymbol{u}_{2,t} \end{array}\right]}_{\boldsymbol{u}_t}$$

$$\boldsymbol{f}_{i,t} = m_i \boldsymbol{g} \quad \text{with} \quad \boldsymbol{g} = \begin{bmatrix} 0 \\ -9.81 \end{bmatrix}$$

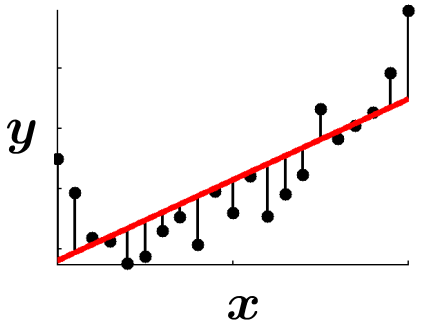
At $t = \frac{T}{2}$ (right hand hitting the ball), we have

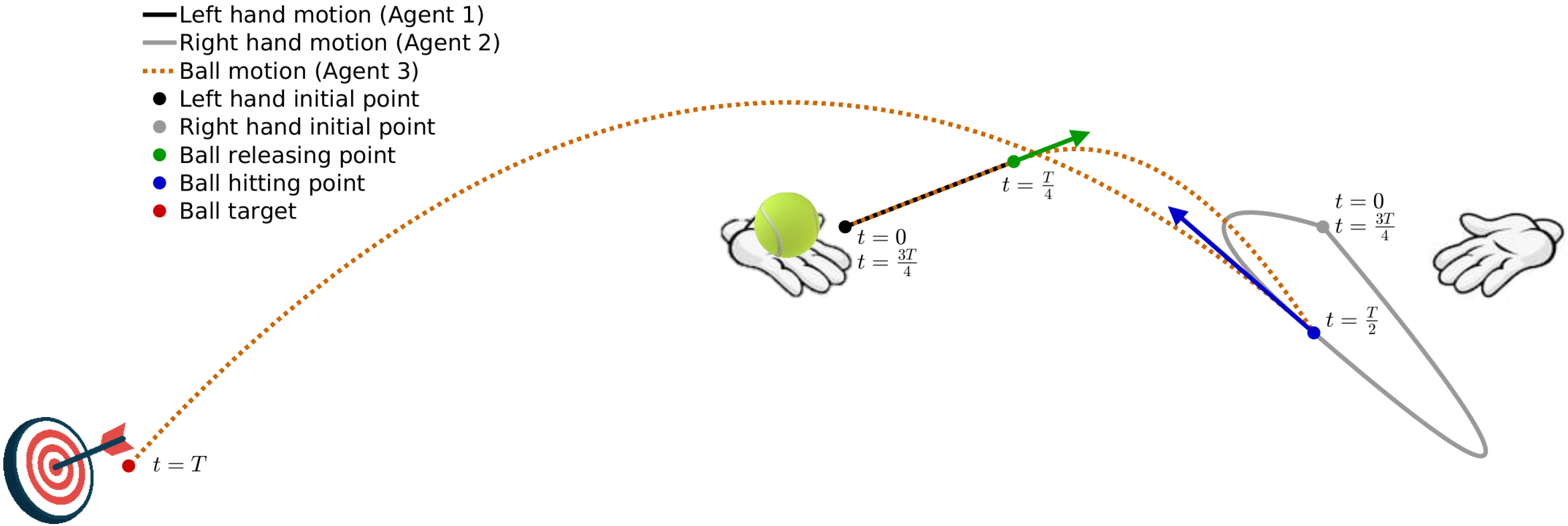
$$\underbrace{\begin{bmatrix} \dot{\mathbf{x}}_{1,t} \\ \ddot{\mathbf{x}}_{1,t} \\ \dot{\boldsymbol{f}}_{1,t} \\ \hline \dot{\mathbf{x}}_{2,t} \\ \ddot{\mathbf{x}}_{2,t} \\ \dot{\boldsymbol{f}}_{2,t} \\ \hline \dot{\mathbf{x}}_{3,t} \\ \ddot{\mathbf{x}}_{3,t} \\ \dot{\boldsymbol{f}}_{3,t} \end{bmatrix}}_{\dot{\boldsymbol{x}}_t} = \underbrace{\left[\begin{array}{ccccccccc} \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{array}\right]}_{\boldsymbol{A}_t^c} \underbrace{\begin{bmatrix} \mathbf{x}_{1,t} \\ \dot{\mathbf{x}}_{1,t} \\ \boldsymbol{f}_{1,t} \\ \hline \mathbf{x}_{2,t} \\ \dot{\mathbf{x}}_{2,t} \\ \boldsymbol{f}_{2,t} \\ \hline \mathbf{x}_{3,t} \\ \dot{\mathbf{x}}_{3,t} \\ \boldsymbol{f}_{3,t} \end{bmatrix}}_{\boldsymbol{x}_t} + \underbrace{\left[\begin{array}{cc} \mathbf{0} & \mathbf{0} \\ \boldsymbol{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I} \\ \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{array}\right]}_{\boldsymbol{B}_t^c} \underbrace{\left[\begin{array}{c} \boldsymbol{u}_{1,t} \\ \hline \boldsymbol{u}_{2,t} \end{array}\right]}_{\boldsymbol{u}_t}$$

For $\frac{T}{4} < t < \frac{T}{2}$ and $t > \frac{T}{2}$ (free motion of the ball), we have

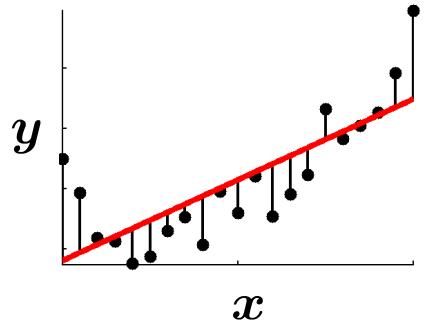
$$\underbrace{\begin{bmatrix} \dot{\mathbf{x}}_{1,t} \\ \ddot{\mathbf{x}}_{1,t} \\ \dot{\boldsymbol{f}}_{1,t} \\ \hline \dot{\mathbf{x}}_{2,t} \\ \ddot{\mathbf{x}}_{2,t} \\ \dot{\boldsymbol{f}}_{2,t} \\ \hline \dot{\mathbf{x}}_{3,t} \\ \ddot{\mathbf{x}}_{3,t} \\ \dot{\boldsymbol{f}}_{3,t} \end{bmatrix}}_{\dot{\boldsymbol{x}}_t} = \underbrace{\left[\begin{array}{ccccccccc} \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{array}\right]}_{\boldsymbol{A}_t^c} \underbrace{\begin{bmatrix} \mathbf{x}_{1,t} \\ \dot{\mathbf{x}}_{1,t} \\ \boldsymbol{f}_{1,t} \\ \hline \mathbf{x}_{2,t} \\ \dot{\mathbf{x}}_{2,t} \\ \boldsymbol{f}_{2,t} \\ \hline \mathbf{x}_{3,t} \\ \dot{\mathbf{x}}_{3,t} \\ \boldsymbol{f}_{3,t} \end{bmatrix}}_{\boldsymbol{x}_t} + \underbrace{\left[\begin{array}{cc} \mathbf{0} & \mathbf{0} \\ \boldsymbol{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I} \\ \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{array}\right]}_{\boldsymbol{B}_t^c} \underbrace{\left[\begin{array}{c} \boldsymbol{u}_{1,t} \\ \hline \boldsymbol{u}_{2,t} \end{array}\right]}_{\boldsymbol{u}_t}$$

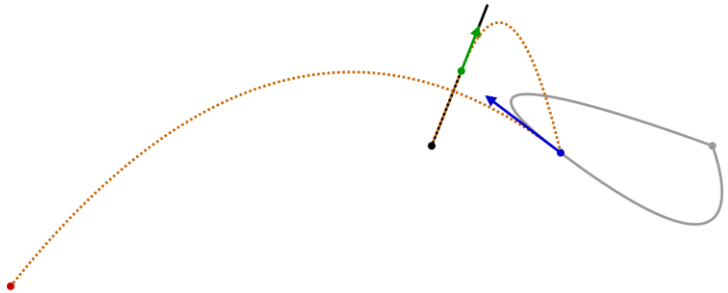
Linear quadratic tracking (LQT) - Example

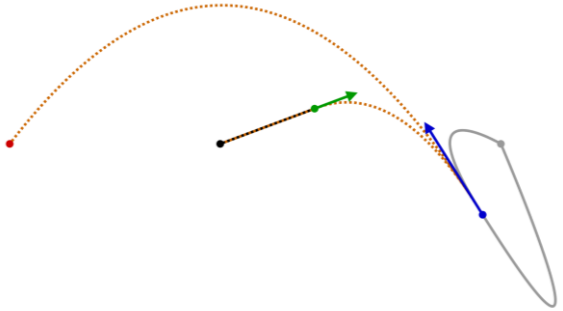


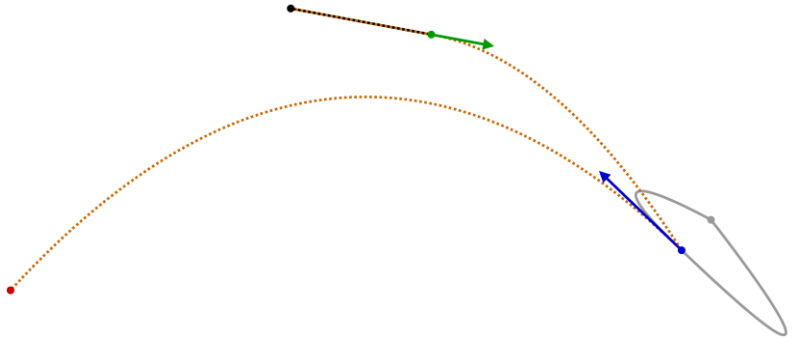


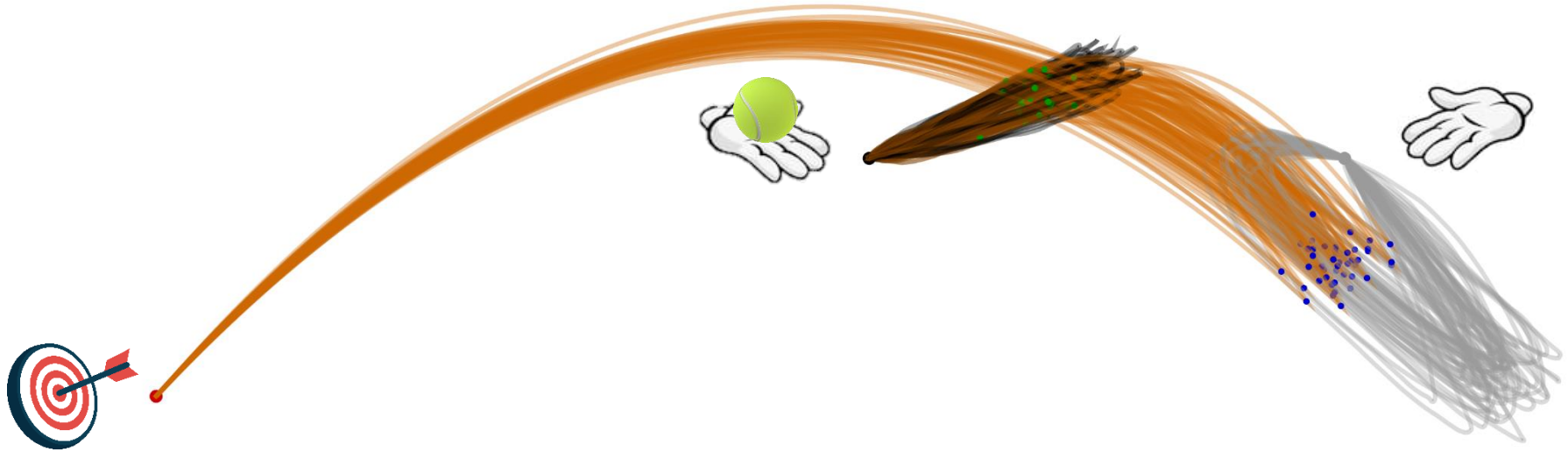
Linear quadratic tracking (LQT) - Example











Logistic regression

Python notebook:
demo_LS_IRLS_logRegr.ipynb

Matlab code:
demo_LS_IRLS_logRegr01.m

Costs functions and associated regression solutions

Univariate output y:

$$\hat{\boldsymbol{a}} = \arg\min_{\boldsymbol{a}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{a}\|^2 \quad = \quad \overbrace{(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top}^{\boldsymbol{X}^\dagger}\, \boldsymbol{y}$$

$$\hat{\boldsymbol{a}} = \arg\min_{\boldsymbol{a}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{a}\|^2_{\mathrm{F},\boldsymbol{W}} \quad = \quad (\boldsymbol{X}^\top \boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}^\top \boldsymbol{W}\, \boldsymbol{y}$$

$$\hat{\boldsymbol{a}} = \arg\min_{\boldsymbol{a}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{a}\|^2_{\mathrm{F}} + \|\boldsymbol{\Gamma}\boldsymbol{a}\|^2_{\mathrm{F}} \quad = \quad (\boldsymbol{X}^\top \boldsymbol{X} + \boldsymbol{\Gamma}^\top\boldsymbol{\Gamma})^{-1}\boldsymbol{X}^\top \boldsymbol{y}$$

$$\hat{\boldsymbol{a}} = \arg\min_{\boldsymbol{a}} f_{\boldsymbol{a}}(\boldsymbol{X}, \boldsymbol{y})$$

Multivariate output y:

$$\hat{\boldsymbol{A}} = \arg\min_{\boldsymbol{A}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|^2 \quad = \quad \overbrace{(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top}^{\boldsymbol{X}^\dagger}\, \boldsymbol{Y}$$

$$\hat{\boldsymbol{A}} = \arg\min_{\boldsymbol{A}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|^2_{\mathrm{F},\boldsymbol{W}} \quad = \quad (\boldsymbol{X}^\top \boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}^\top \boldsymbol{W}\, \boldsymbol{Y}$$

$$\hat{\boldsymbol{A}} = \arg\min_{\boldsymbol{A}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|^2_{\mathrm{F}} + \|\boldsymbol{\Gamma}\boldsymbol{A}\|^2_{\mathrm{F}} \quad = \quad (\boldsymbol{X}^\top \boldsymbol{X} + \boldsymbol{\Gamma}^\top\boldsymbol{\Gamma})^{-1}\boldsymbol{X}^\top \boldsymbol{Y}$$

Logistic regression

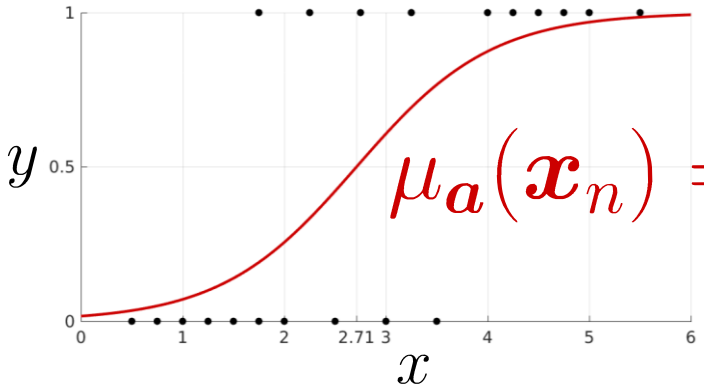
Bernoulli distribution *(for binary variables)*:

$$\mathcal{L}_n = \begin{cases} \overbrace{p}^{\mathcal{P}(y_n=1)} & \text{if } y_n = 1, \\ \underbrace{1-p}_{\mathcal{P}(y_n=0)} & \text{if } y_n = 0. \end{cases}$$

$$= p^{y_n} \, (1-p)^{(1-y_n)}$$

Logistic function:

$$y_n \in \{0, 1\}$$



$$\mu_{\boldsymbol{a}}(\boldsymbol{x}_n) = \frac{1}{1+e^{-\boldsymbol{a}^\intercal \boldsymbol{x}_n}}$$

Likelihood of *n*th datapoint:

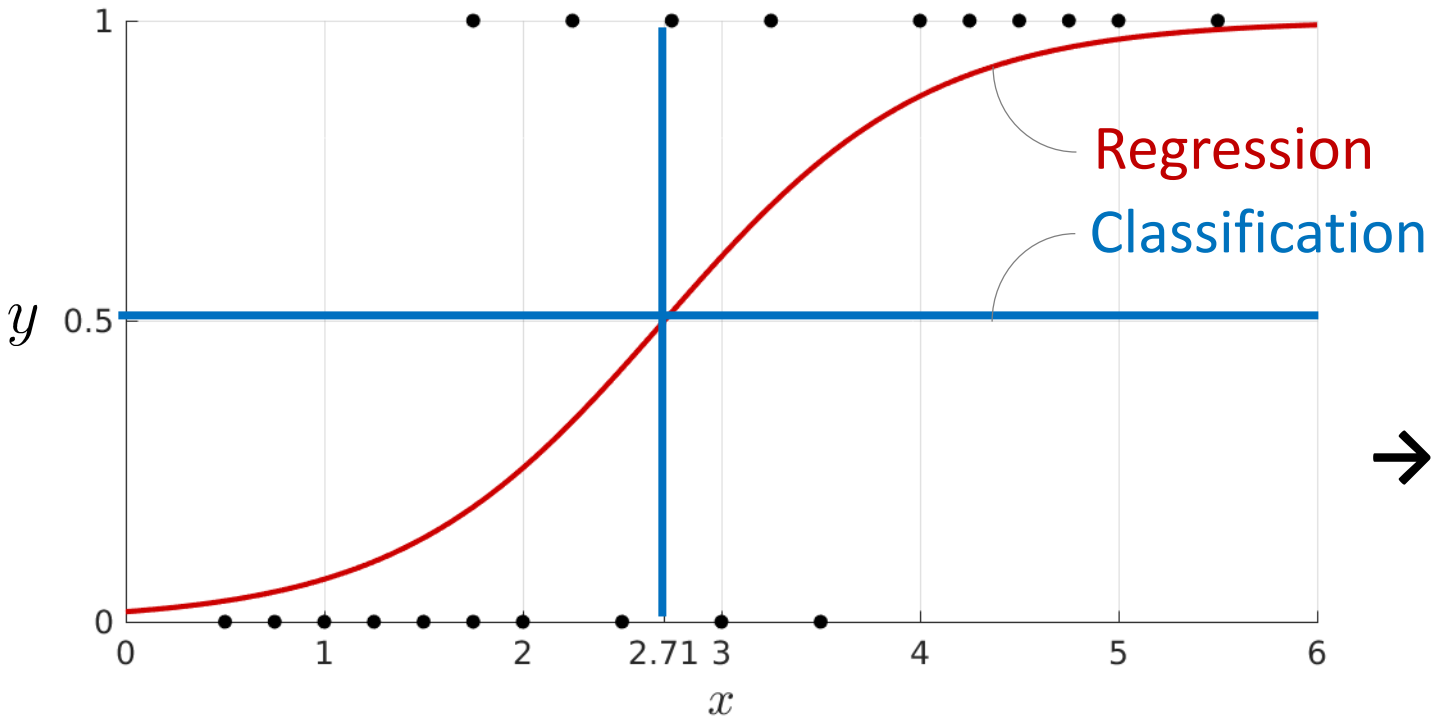
$$\mathcal{L}_n = \mu_{\boldsymbol{a}}(\boldsymbol{x}_n)^{y_n} \big(1 - \mu_{\boldsymbol{a}}(\boldsymbol{x}_n)\big)^{(1-y_n)}$$

Likelihood of N datapoints *(independence assumption)*:

$$\mathcal{L} = \prod_n \mu_{\boldsymbol{a}}(\boldsymbol{x}_n)^{y_n} \big(1 - \mu_{\boldsymbol{a}}(\boldsymbol{x}_n)\big)^{(1-y_n)}$$

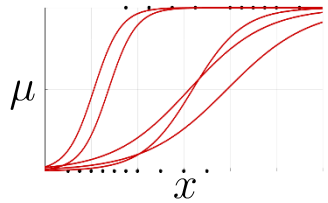
Logistic regression

Pass/fail in function of the time spent to study at an exam:



→ **Regression exploited for classification problem**

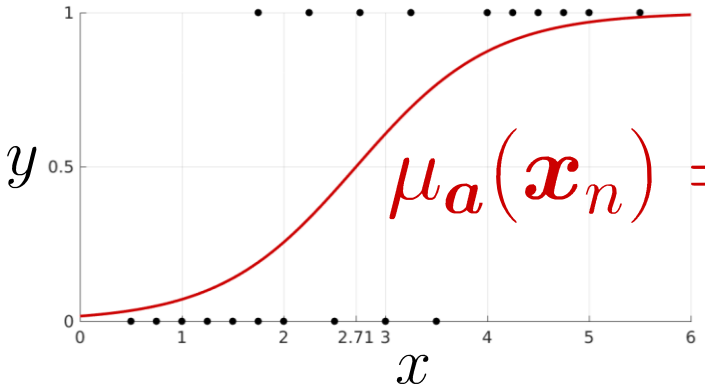
Logistic function:



$$\mu_{\boldsymbol{a}}(\boldsymbol{x}) = \frac{1}{1+e^{-\boldsymbol{a}^\top \boldsymbol{x}}} \qquad \mu_{\boldsymbol{a}}(x) = \frac{1}{1+e^{-(a_1+a_2 x)}}$$

Logistic regression

$y_n \in \{0, 1\}$



$$\mu_{\boldsymbol{a}}(\boldsymbol{x}_n) = \frac{1}{1+e^{-\boldsymbol{a}^\top \boldsymbol{x}_n}}$$

Likelihood of N datapoints:

$$\mathcal{L} = \prod_n \mu_{\boldsymbol{a}}(\boldsymbol{x}_n)^{y_n} \left(1 - \mu_{\boldsymbol{a}}(\boldsymbol{x}_n)\right)^{(1-y_n)}$$

Cost function as negative log-likelihood:

$\log(a^b) = b\log(a)$ — $\log(ab) = \log(a) + \log(b)$

$$c = -\sum_n y_n \log\left(\mu_{\boldsymbol{a}}(\boldsymbol{x}_n)\right) + (1 - y_n) \log\left(1 - \mu_{\boldsymbol{a}}(\boldsymbol{x}_n)\right)$$

$\frac{\partial}{\partial x}\log(x) = \frac{1}{x}$

$$\frac{\partial c}{\partial \boldsymbol{a}} = -\sum_n y_n \, \mu_{\boldsymbol{a}}^{-1} \mu_{\boldsymbol{a}} \left(1 - \mu_{\boldsymbol{a}}\right) \boldsymbol{x}_n - (1 - y_n)(1 - \mu_{\boldsymbol{a}})^{-1} \mu_{\boldsymbol{a}} \left(1 - \mu_{\boldsymbol{a}}\right) \boldsymbol{x}_n$$

$$= -\sum_n y_n \left(1 - \mu_{\boldsymbol{a}}\right) \boldsymbol{x}_n - \left(1 - y_n\right) \mu_{\boldsymbol{a}} \, \boldsymbol{x}_n$$

$$= \sum_n (\mu_{\boldsymbol{a}} - y_n) \, \boldsymbol{x}_n$$

$$\mu(x) = \frac{1}{1+e^{-x}}$$

$$\frac{\partial \mu}{\partial x} = \mu(1 - \mu)$$

Logistic regression

$$\frac{\partial c}{\partial \boldsymbol{a}} = \sum_n (\mu_{\boldsymbol{a}} - y_n)\boldsymbol{x}_n$$

$$\mu_{\boldsymbol{a}}(\boldsymbol{x}_n) = \frac{1}{1+e^{-\boldsymbol{a}^\top \boldsymbol{x}_n}}$$

It can for example be solved with Newton's method, by iterating

$$\boldsymbol{a} \leftarrow \boldsymbol{a} - \boldsymbol{H}^{-1}\boldsymbol{g},$$

with gradient $\boldsymbol{g} = \sum_n (\mu_{\boldsymbol{a}}(\boldsymbol{x}_n) - y_n)\boldsymbol{x}_n = \boldsymbol{X}^\top(\boldsymbol{\mu}_{\boldsymbol{a}} - \boldsymbol{y})$ and Hessian $\boldsymbol{H} = \boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X}$,
with diagonal matrix $\boldsymbol{W} = \mathrm{diag}\big(\boldsymbol{\mu}_{\boldsymbol{a}} * (\boldsymbol{1} - \boldsymbol{\mu}_{\boldsymbol{a}})\big)$.

$*$ Hadamard (elementwise) product

We then obtain

$$\begin{aligned}
\boldsymbol{a} &\leftarrow \boldsymbol{a} - \boldsymbol{H}^{-1}\boldsymbol{g} \\
&\leftarrow \boldsymbol{a} - (\boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X})^{-1}\boldsymbol{X}^\top(\boldsymbol{\mu}_{\boldsymbol{a}} - \boldsymbol{y}) \\
&\leftarrow (\boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X})^{-1}\big(\boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X}\boldsymbol{a} - \boldsymbol{X}^\top(\boldsymbol{\mu}_{\boldsymbol{a}} - \boldsymbol{y})\big) \\
&\leftarrow (\boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X})^{-1}\boldsymbol{X}^\top(\boldsymbol{W}\boldsymbol{X}\boldsymbol{a} + \boldsymbol{y} - \boldsymbol{\mu}_{\boldsymbol{a}}) \\
&\leftarrow (\boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X})^{-1}\boldsymbol{X}^\top \boldsymbol{W}\boldsymbol{z},
\end{aligned}$$

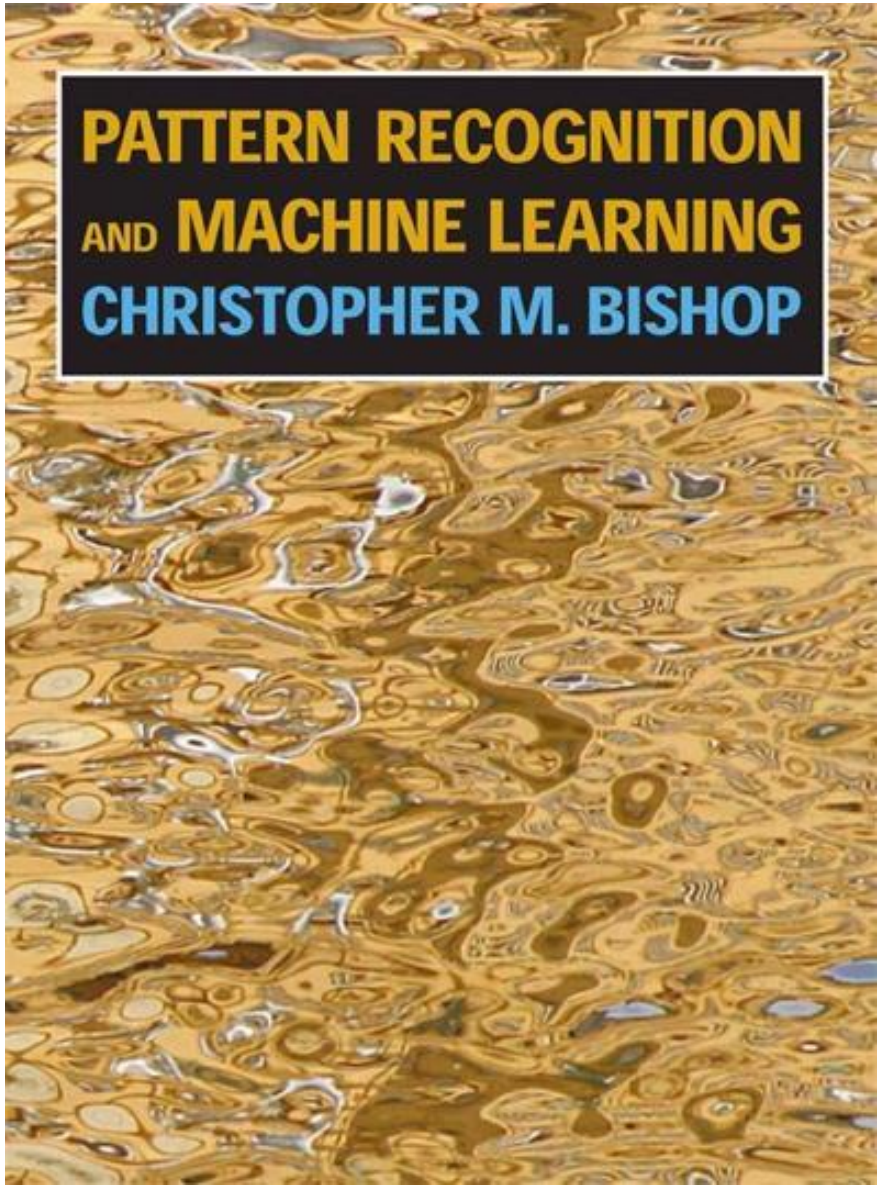
with *working response* $\boldsymbol{z} = \boldsymbol{X}\boldsymbol{a} + \boldsymbol{W}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}_{\boldsymbol{a}})$.

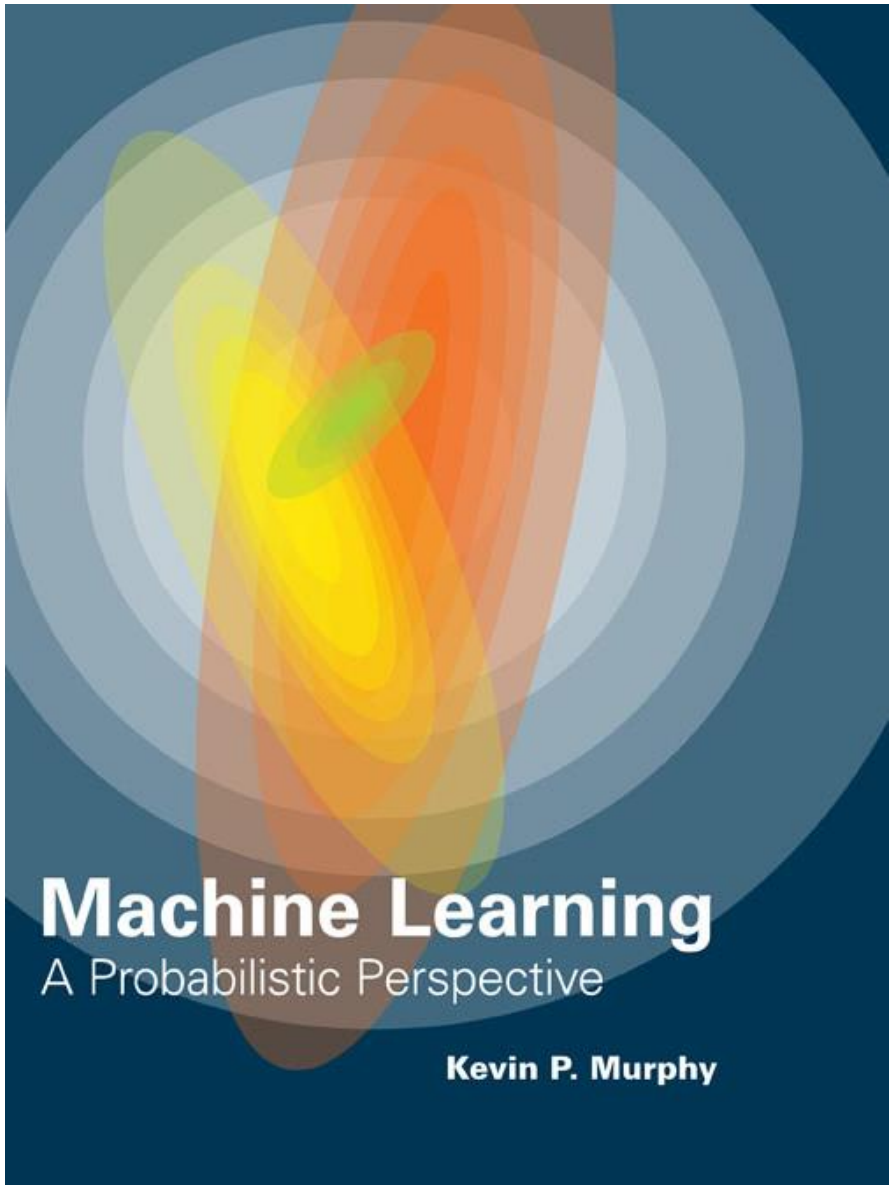
$$\mu(x) = \frac{1}{1+e^{-x}}$$

$$\frac{\partial \mu}{\partial x} = \mu(1-\mu)$$

→ IRLS algorithm

Recommended reading material





The Matrix Cookbook

Kaare Brandt Petersen
Michael Syskind Pedersen

Labs this afternoon

https://moodle.epfl.ch/course/view.php?id=16819

INM11, 14:15-16:00

Dr João Silvério