

Scalable Non-Parametric Statistical Estimation

Aymeric DIEULEVEUT

ENS Paris, INRIA

February 6, 2017



Statistics

Statistical model

Performance measure

Estimator

Convergence: $F(\#obs)$

Statistics

Statistical model

Performance measure

Estimator

Convergence: $F(\#obs)$

Optimization

Minimize a given function

Algorithm focused

Scales with dimension and observations

Convergence: $F(\#iter)$

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$



Accurate & Efficient

Scalable estimators with
optimal statistical properties



Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Non-parametric
Regression
Square loss
Tikhonov regularization

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Non-parametric
Regression
Square loss
Tikhonov regularization

Stochastic
algorithms
First order methods
Few passes on the data

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Non-parametric
Regression
Square loss
Tikhonov regularization

Non-parametric
Stochastic
Approximation,
AOS, 2015

Stochastic
algorithms
First order methods
Few passes on the data

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression.

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression.

$$\varepsilon(f) := \mathbb{E}_{(X,Y)} \left[(f(X) - Y)^2 \right].$$

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression.

$$\varepsilon(f) := \mathbb{E}_{(X,Y)} \left[(f(X) - Y)^2 \right].$$

Within a reproducing kernel Hilbert space \mathcal{H} :

$$\min_{f \in \mathcal{H}} \varepsilon(f).$$

(x_i, y_i) i.i.d. observations.

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression. Sequence of estimators $f_t \in \mathcal{H}$.

$$\varepsilon(f) := \mathbb{E}_{(X,Y)} \left[(f(X) - Y)^2 \right].$$

Within a reproducing kernel Hilbert space \mathcal{H} :

$$\min_{f \in \mathcal{H}} \varepsilon(f).$$

(x_i, y_i) i.i.d. observations.

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression.

$$\varepsilon(f) := \mathbb{E}_{(X,Y)} \left[(f(X) - Y)^2 \right].$$

Within a reproducing kernel Hilbert space \mathcal{H} :

$$\min_{f \in \mathcal{H}} \varepsilon(f).$$

(x_i, y_i) i.i.d. observations.

Sequence of estimators $f_t \in \mathcal{H}$.

Update after each observation.

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression.

$$\varepsilon(f) := \mathbb{E}_{(X,Y)} \left[(f(X) - Y)^2 \right].$$

Within a reproducing kernel Hilbert space \mathcal{H} :

$$\min_{f \in \mathcal{H}} \varepsilon(f).$$

(x_i, y_i) i.i.d. observations.

Sequence of estimators $f_t \in \mathcal{H}$.

Update after each observation.

Using unbiased gradients of the loss function:

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression.

$$\varepsilon(f) := \mathbb{E}_{(X,Y)} \left[(f(X) - Y)^2 \right].$$

Within a reproducing kernel Hilbert space \mathcal{H} :

$$\min_{f \in \mathcal{H}} \varepsilon(f).$$

(x_i, y_i) i.i.d. observations.

Sequence of estimators $f_t \in \mathcal{H}$.

Update after each observation.

Using unbiased gradients of the loss function:

$$f_{t+1} = f_t - \gamma_t (f_t(x_t) - y_t) K_{x_t},$$

where: K is the kernel,

$$K_x = K(x, \cdot).$$

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression.

$$\varepsilon(f) := \mathbb{E}_{(X,Y)} \left[(f(X) - Y)^2 \right].$$

Within a reproducing kernel Hilbert space \mathcal{H} :

$$\min_{f \in \mathcal{H}} \varepsilon(f).$$

(x_i, y_i) i.i.d. observations.

Sequence of estimators $f_t \in \mathcal{H}$.

Update after each observation.

Using unbiased gradients of the loss function:

$$f_{t+1} = f_t - \gamma_t (f_t(x_t) - y_t) K_{x_t},$$

where: K is the kernel,

$$K_x = K(x, \cdot).$$

↔ Stochastic Approximation.

Non-parametric Stochastic Approximation with large step sizes 1/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.

Random design least-squares regression.

$$\varepsilon(f) := \mathbb{E}_{(X,Y)} \left[(f(X) - Y)^2 \right].$$

Within a reproducing kernel Hilbert space \mathcal{H} :

$$\min_{f \in \mathcal{H}} \varepsilon(f).$$

(x_i, y_i) i.i.d. observations.

Sequence of estimators $f_t \in \mathcal{H}$.

Update after each observation.

Using unbiased gradients of the loss function:

$$f_{t+1} = f_t - \gamma_t (f_t(x_t) - y_t) K_{x_t},$$

where: K is the kernel,

$$K_x = K(x, \cdot).$$

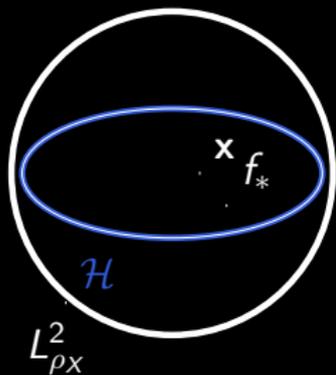
↪ Stochastic Approximation.

Depending on assumptions on:

- ▶ the Gaussian complexity of the unit ball of the kernel space,
- ▶ the smoothness in \mathcal{H} of the optimal predictor $f_*(X) = \mathbb{E}[Y|X]$.

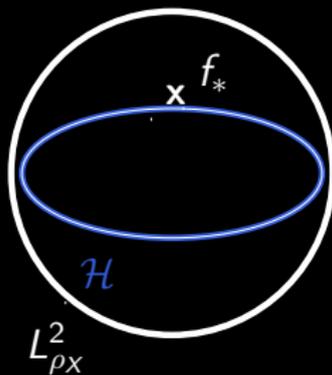
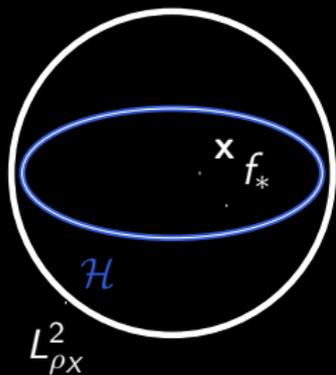
Non-parametric Stochastic Approximation with large step sizes 2/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.



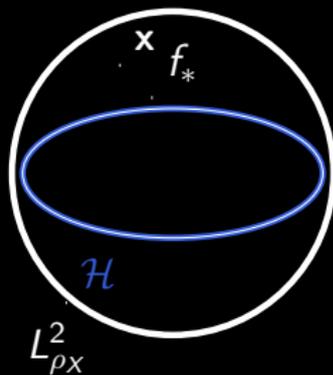
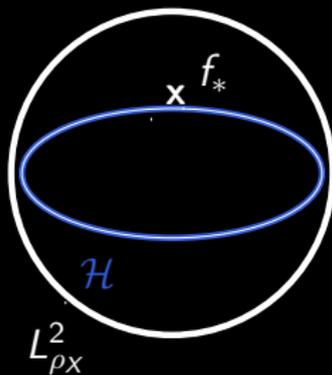
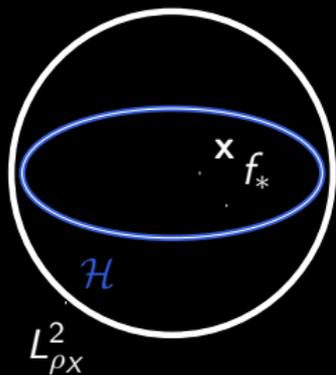
Non-parametric Stochastic Approximation with large step sizes 2/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.



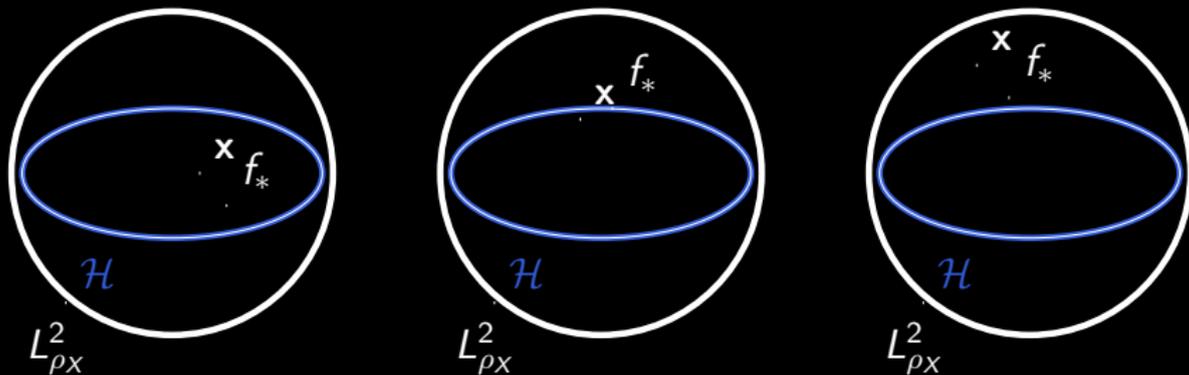
Non-parametric Stochastic Approximation with large step sizes 2/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.



Non-parametric Stochastic Approximation with large step sizes 2/2.

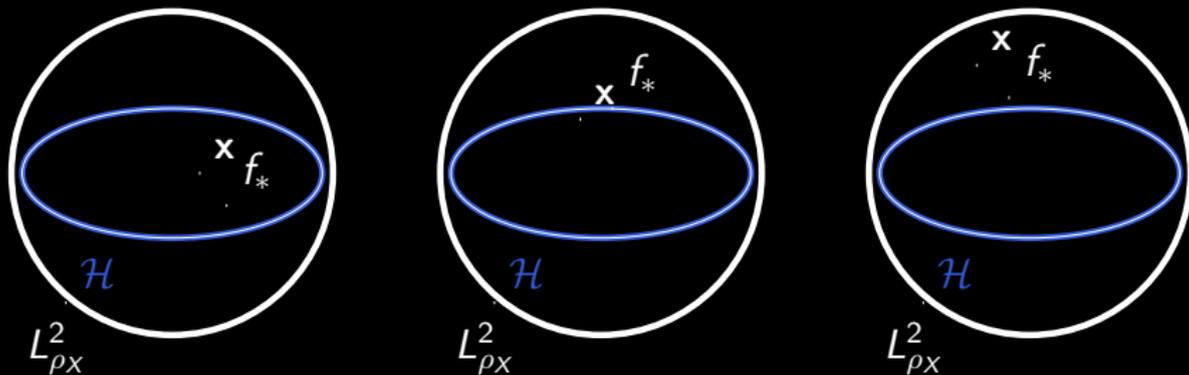
Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.



Theorem: Averaged, unregularized, least mean squares algorithm, with large step sizes, gets Statistical optimal rate of convergence.

Non-parametric Stochastic Approximation with large step sizes 2/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.



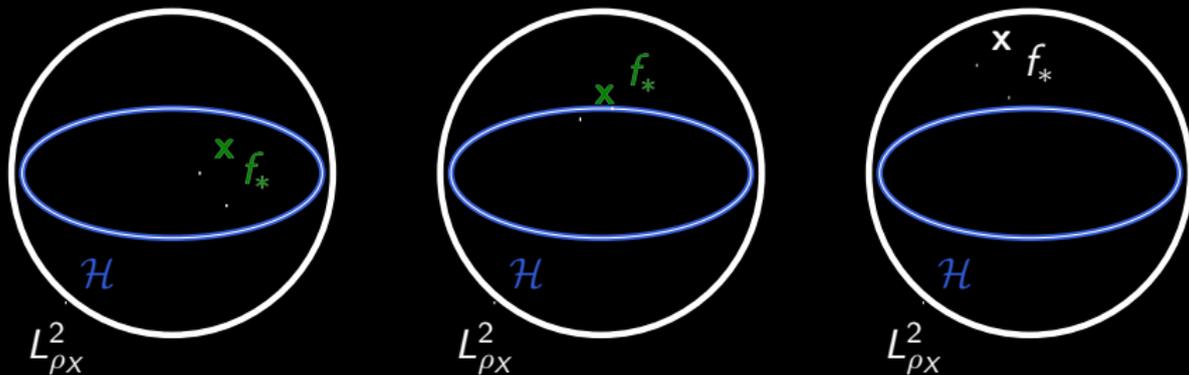
Theorem: Averaged, unregularized, least mean squares algorithm, with large step sizes, gets Statistical optimal rate of convergence.

↪ Recovers the finite dimension situation with rate $O\left(\frac{\sigma^2 d}{n}\right)$.

↪ Optimal rates in both the well-specified regime and some situations of the mis-specified.

Non-parametric Stochastic Approximation with large step sizes 2/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.



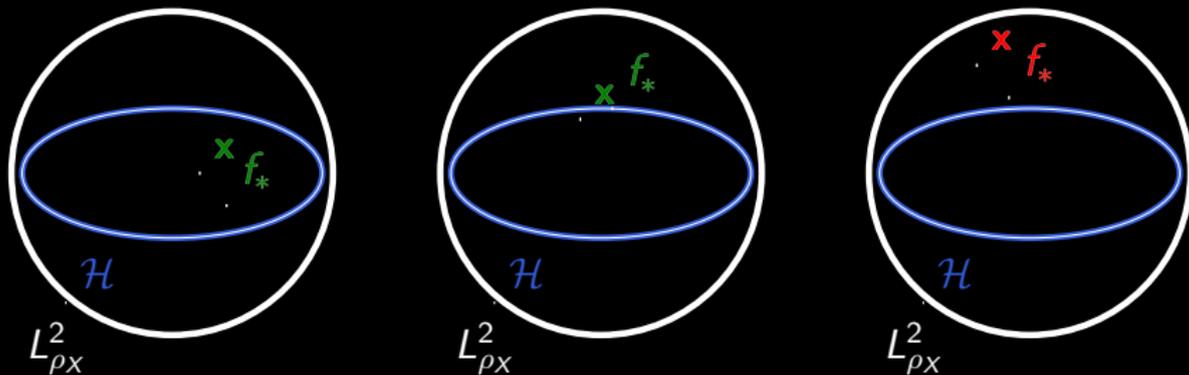
Theorem: Averaged, unregularized, least mean squares algorithm, with large step sizes, gets Statistical optimal rate of convergence.

↪ Recovers the finite dimension situation with rate $O\left(\frac{\sigma^2 d}{n}\right)$.

↪ Optimal rates in both the well-specified regime and some situations of the mis-specified.

Non-parametric Stochastic Approximation with large step sizes 2/2.

Aymeric Dieuleveut & Francis Bach, *in the Annals of Statistics*, 2015.



Theorem: Averaged, unregularized, least mean squares algorithm, with large step sizes, gets Statistical optimal rate of convergence.

↪ Recovers the finite dimension situation with rate $O\left(\frac{\sigma^2 d}{n}\right)$.

↪ Optimal rates in both the well-specified regime and some situations of the mis-specified.

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Non-parametric
Regression
Square loss
Tikhonov regularization

Non-parametric
Stochastic
Approximation,
AOS, 2015

Stochastic
algorithms
First order methods
Few passes on the data

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Non-parametric
Regression
Square loss
Tikhonov regularization

Non-parametric
Stochastic
Approximation,
AOS, 2015

Stochastic
algorithms
First order methods
Few passes on the data

Faster Rates for
Least-Squares Regression,
Tech. report, 2016

Harder, Better, Faster, Stronger Convergence Rates for Least Squares Regression

Aymeric Dieuleveut, Nicolas Flammarion & Francis Bach, Technical report, 2016.

Classical tradeoff: a **Bias term** and a **Variance term** appear.

- ▶ The bias is the hardness of forgetting the initial condition.
- ▶ The variance is linked with the statistical hardness of the problem.

Harder, Better, Faster, Stronger Convergence Rates for Least Squares Regression

Aymeric Dieuleveut, Nicolas Flammarion & Francis Bach, Technical report, 2016.

Classical tradeoff: a **Bias term** and a **Variance term** appear.

- ▶ The bias is the hardness of forgetting the initial condition.
- ▶ The variance is linked with the statistical hardness of the problem.

Lower bounds:

- ▶ Optimal first order algorithm forgets initial conditions as $\Omega\left(\frac{\|\theta_0 - \theta_*\|^2}{t^2}\right)$
- ▶ Optimal statistical estimation is $\Omega\left(\frac{\sigma^2 d}{n}\right)$,

Harder, Better, Faster, Stronger Convergence Rates for Least Squares Regression

Aymeric Dieuleveut, Nicolas Flammarion & Francis Bach, Technical report, 2016.

Classical tradeoff: a **Bias term** and a **Variance term** appear.

- ▶ The bias is the hardness of forgetting the initial condition.
- ▶ The variance is linked with the statistical hardness of the problem.

Lower bounds:

- ▶ Optimal first order algorithm forgets initial conditions as $\Omega\left(\frac{\|\theta_0 - \theta_*\|^2}{t^2}\right)$
- ▶ Optimal statistical estimation is $\Omega\left(\frac{\sigma^2 d}{n}\right)$,
- ▶ Single pass over the data: $t = n$.

Harder, Better, Faster, Stronger Convergence Rates for Least Squares Regression

Aymeric Dieuleveut, Nicolas Flammarion & Francis Bach, Technical report, 2016.

Classical tradeoff: a **Bias term** and a **Variance term** appear.

- ▶ The bias is the hardness of forgetting the initial condition.
- ▶ The variance is linked with the statistical hardness of the problem.

Lower bounds:

- ▶ Optimal first order algorithm forgets initial conditions as $\Omega\left(\frac{\|\theta_0 - \theta_*\|^2}{t^2}\right)$
- ▶ Optimal statistical estimation is $\Omega\left(\frac{\sigma^2 d}{n}\right)$,
- ▶ Single pass over the data: $t = n$.

New algorithm, based on Nesterov acceleration:

- ↪ Both optimal terms: $\mathbb{E} [\varepsilon(\bar{\theta}_n) - \varepsilon(\bar{\theta}_*)] \leq \frac{L\|\theta_0 - \theta_*\|^2}{n^2} + \frac{\sigma^2 d}{n}$.
- ↪ Improves convergence rate for mis-specified non-parametric regression.

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Non-parametric
Regression
Square loss
Tikhonov regularization

Non-parametric
Stochastic
Approximation,
AOS, 2015

Stochastic
algorithms
First order methods
Few passes on the data

Faster Rates for
Least-Squares Regression,
Tech. report, 2016

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Non-parametric
Regression
Square loss
Tikhonov regularization

Non-parametric
Stochastic
Approximation,
AOS, 2015

Stochastic
algorithms
First order methods
Few passes on the data

Adaptation to the
smoothness for learning
in Kernel spaces

Faster Rates for
Least-Squares Regression,
Tech. report, 2016

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$



Accurate & Efficient

Scalable estimators with
optimal statistical properties



Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Density estimation
Shape constraint
(log concave)
MLE

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Density estimation
Shape constraint
(log concave)
MLE

Non smooth
optimization

Statistics

Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient

Scalable estimators with
optimal statistical properties

Optimization

Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Density estimation
Shape constraint
(log concave)
MLE

New ideas

Non smooth
optimization

Statistics
Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient
Scalable estimators with
optimal statistical properties

Optimization
Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Density estimation
Shape constraint
(log concave)
MLE

Non smooth
optimization



New ideas



Scalable MLE algorithm in
high dimension ?

Statistics
Statistical model
Performance measure
Estimator
Convergence: $F(\#obs)$

Accurate & Efficient
Scalable estimators with
optimal statistical properties

Optimization
Minimize a given function
Algorithm focused
Scales with dimension and
observations
Convergence: $F(\#iter)$

Density estimation
Shape constraint
(log concave)
MLE

Non smooth
optimization



Online algorithm ?

Scalable MLE algorithm in
high dimension ?