Statsitical Analysis of On-line Learning

optimal and semi-optimal stochastic gradient

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June 9, 2023

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Introduction

notation:

- data: i.i.d.~ observations from ground truth distribution P

$$z_1, z_2, \ldots, z_t, \ldots \sim^{\text{i.i.d.}} P$$

- learning machine: specified by a finite dimensional parameter

$$\theta \in \Theta \subset \mathbb{R}^m$$

- loss function: penalty of machine θ for a given datum z

$$l(z;\theta) \quad \text{(a smooth function with respect to } \theta\text{)}$$

for example:

$$l(z;\theta) = -\log p(z:\theta) \qquad \text{negative log loss}$$
$$l(z;\theta) = |y - f(x;\theta)|^2 \qquad \text{squared loss for } z = (x, y)$$

- population loss: not accessible

$$L(\theta) = \mathbb{E}_{Z\sim P}[l(Z;\theta)]$$

$$\theta = \arg\min_{\theta} L(\theta) \quad \text{(optimal parameter)}$$

- empirical loss: accessible

$$\hat{L}_t(\theta) = \frac{1}{t}\sum_{z_i \in D_t} l(z_i;\theta), \quad D_t = \{z_i; i = 1, \ldots, t\}$$

- $\hat{L}$ is justified by *the law of large numbers*

$$\hat{L}_t(\theta) = \frac{1}{t}\sum_{z_i \in D_t} l(z_i;\theta) \xrightarrow{t\to\infty} L(\theta) = \mathbb{E}_{Z\sim P}\left[l(Z;\theta)\right]$$

- batch learning: minimize the empirical loss

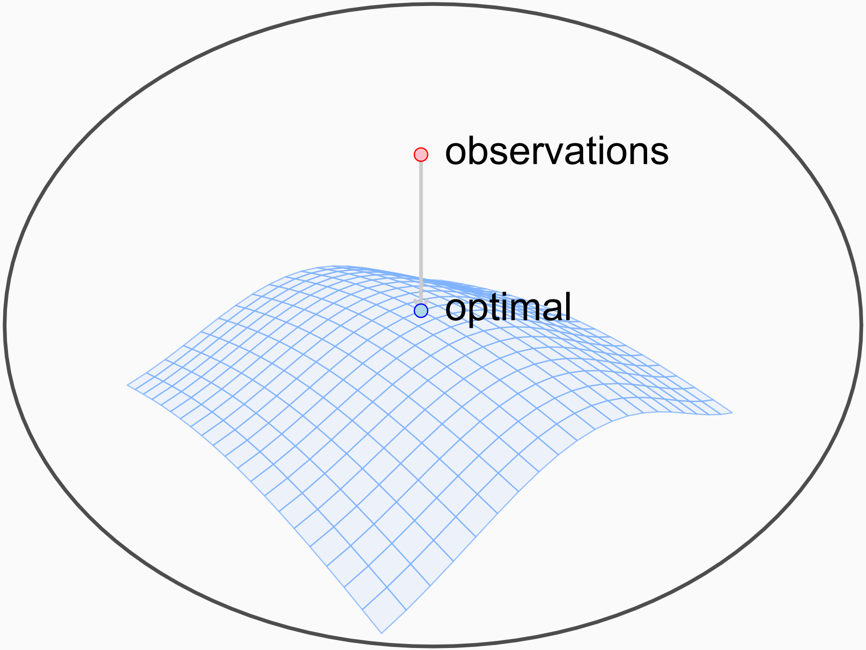
$$\hat{\theta}_t = \arg\min_{\theta} \hat{L}_t(\theta),$$

- on-line learning: update sequentially with a datum sampled at each time (or resampled from pooled data)

$$\theta_t = \theta_{t-1} - \Phi_t \nabla l(z_t; \theta_{t-1}),$$

where ∇ denotes the gradient with respect to θ, and Φ is a matrix which controls the rate of convergence.

- batch learning:
  - pros:: can adopt wide class of loss functions
  - cons:: shows slow convergence
    may have many local minima
    should store all the observations
- on-line learning:
  - pros:: do not have to store all the observations
    (good for massive data stream)
    can escape from local minima
    can follow the change of true distributions
  - cons:: should control learning rate ε properly
    (do not converge with constant ε)


observations
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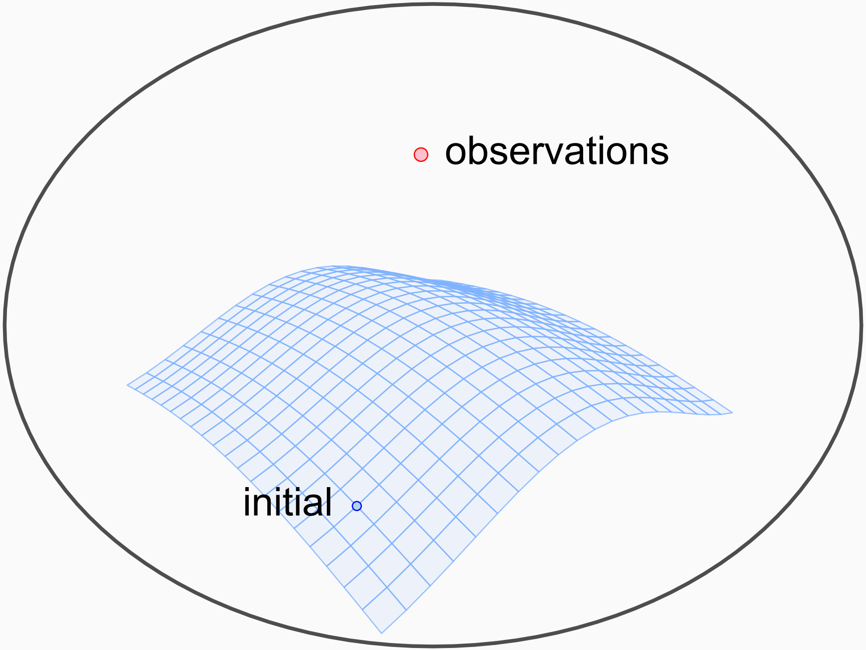
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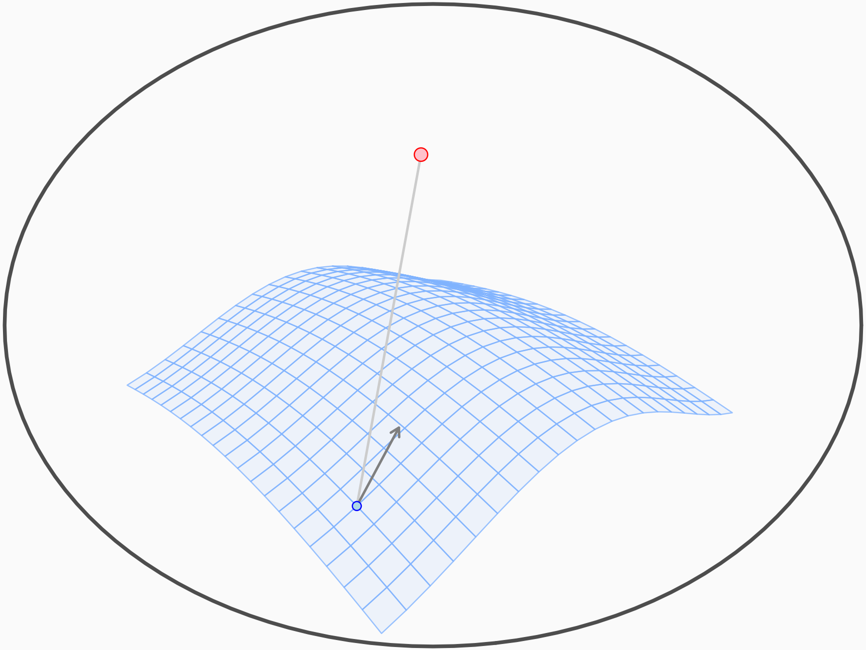
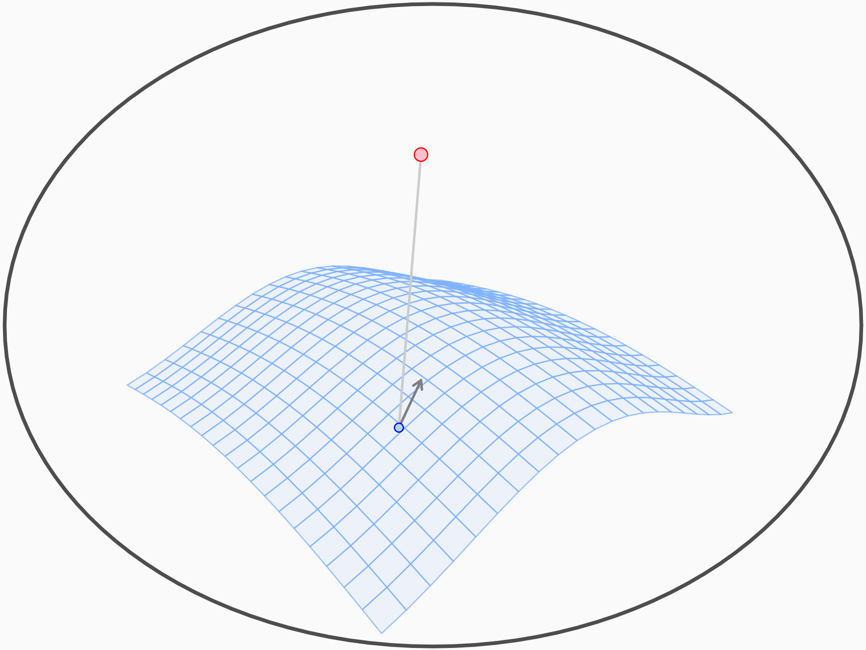
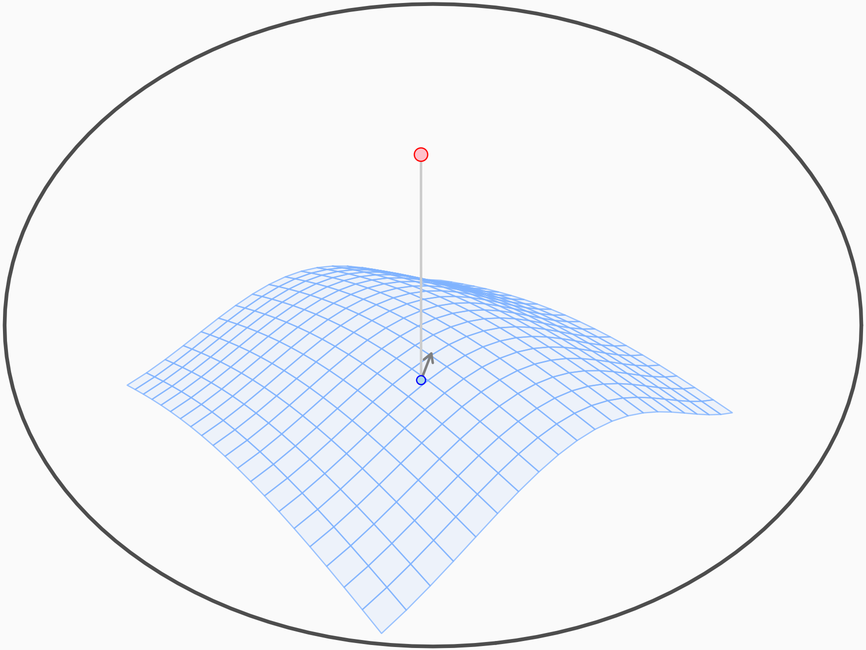
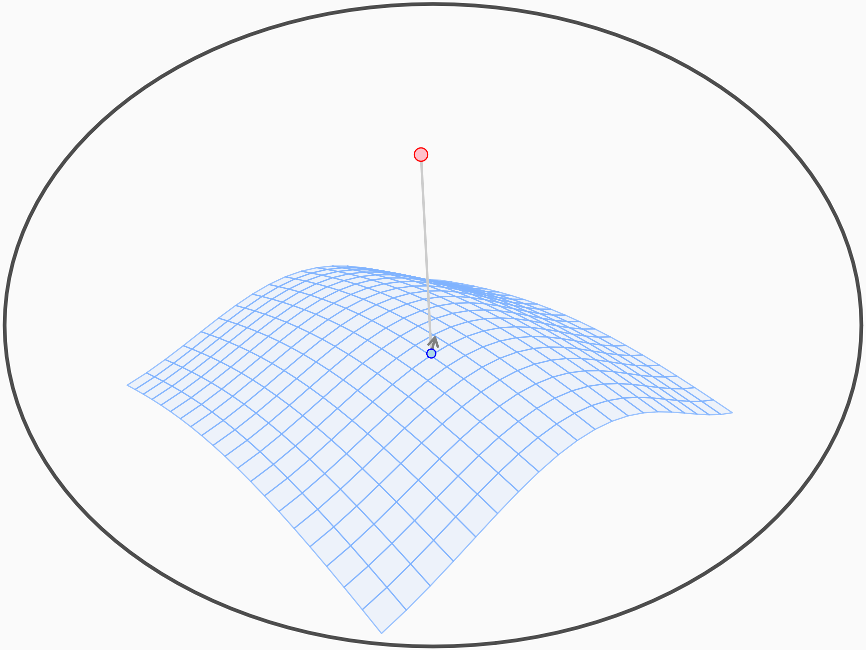
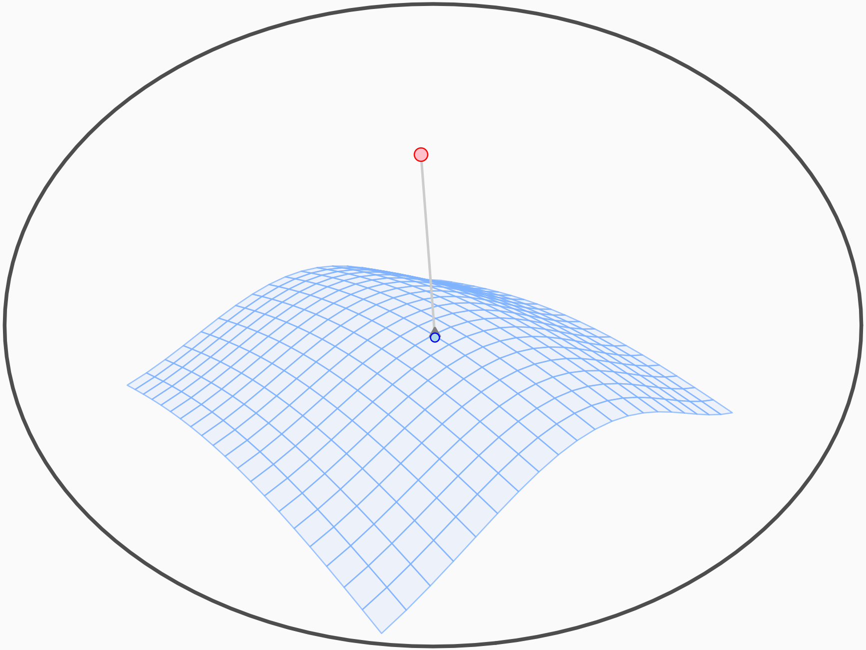
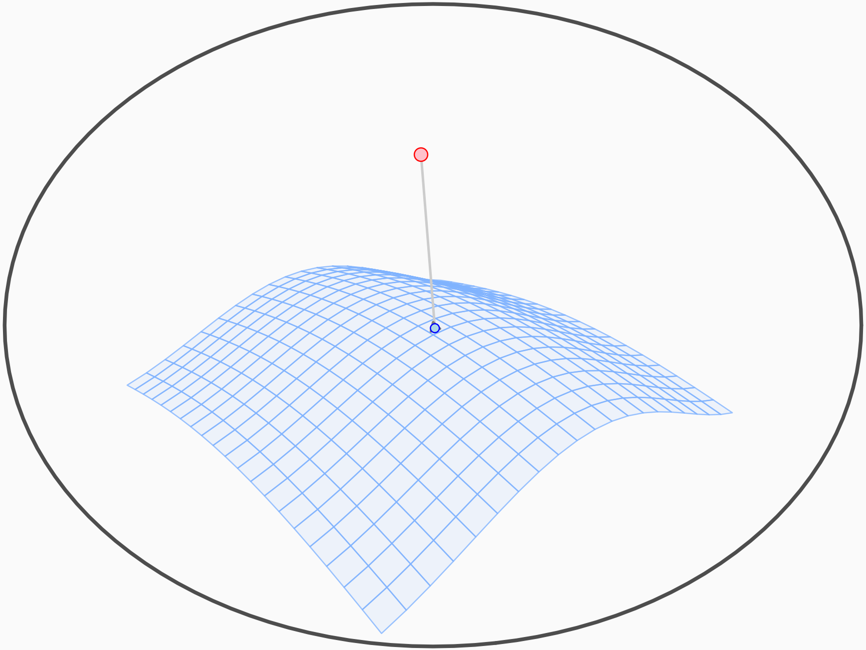


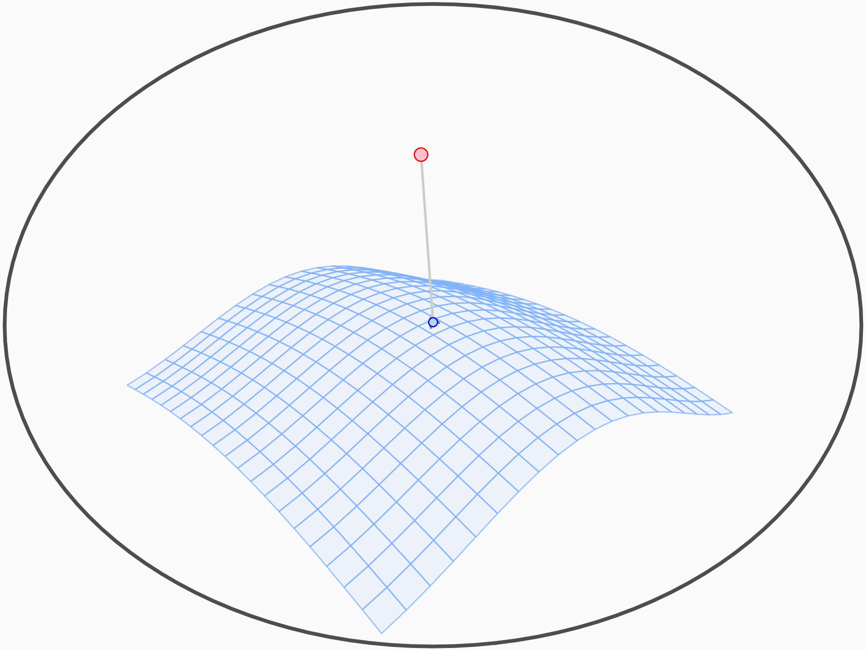


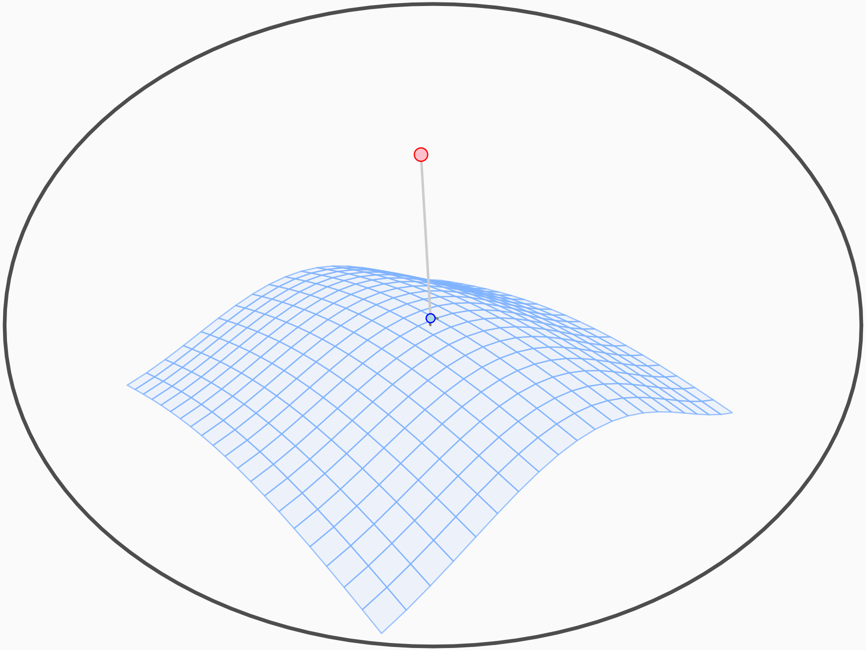


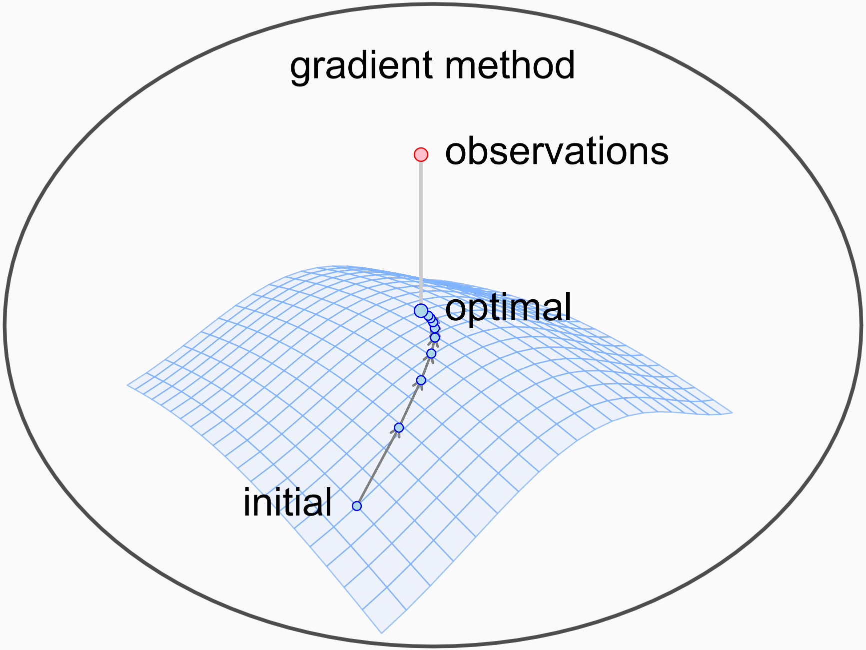


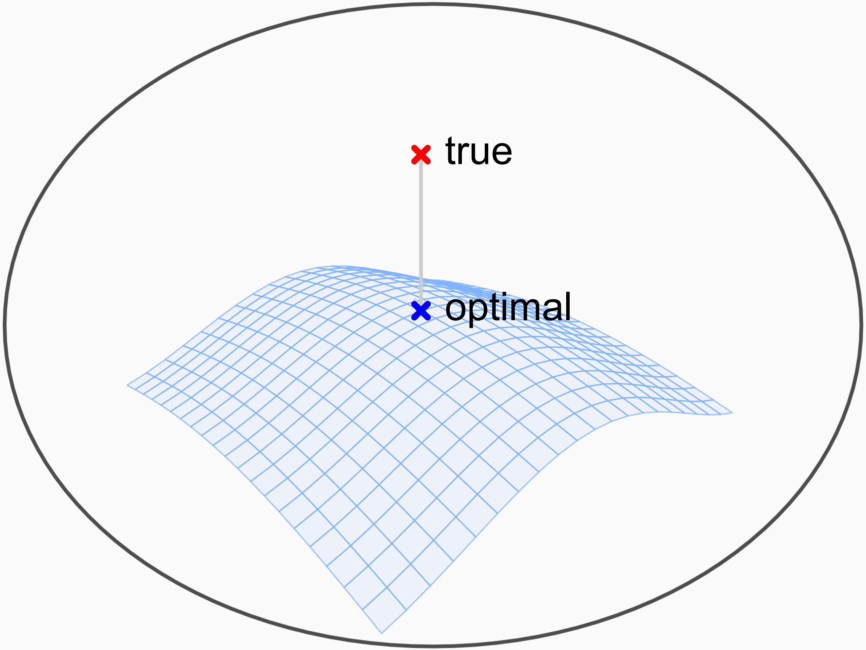









gradient method
observations
optimal
initial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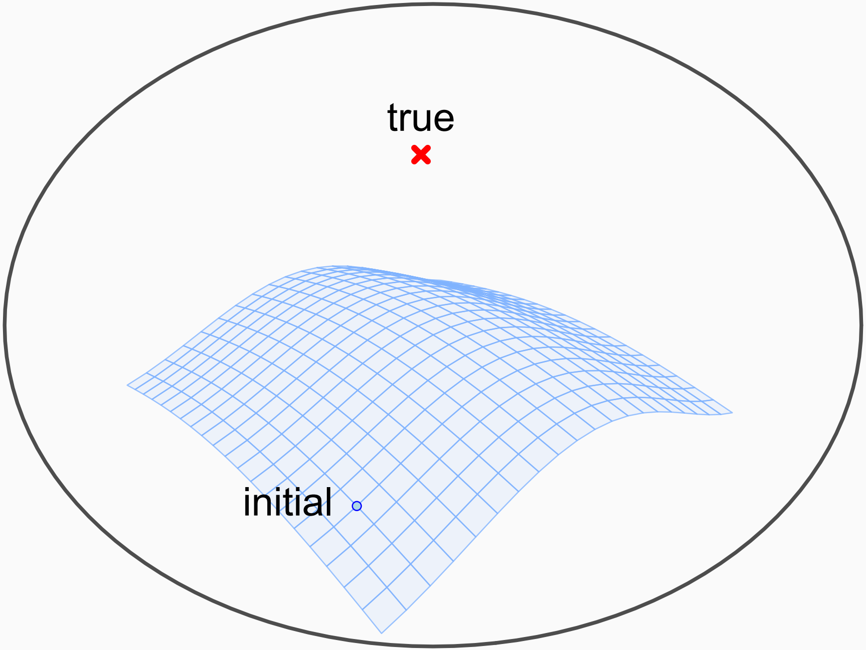
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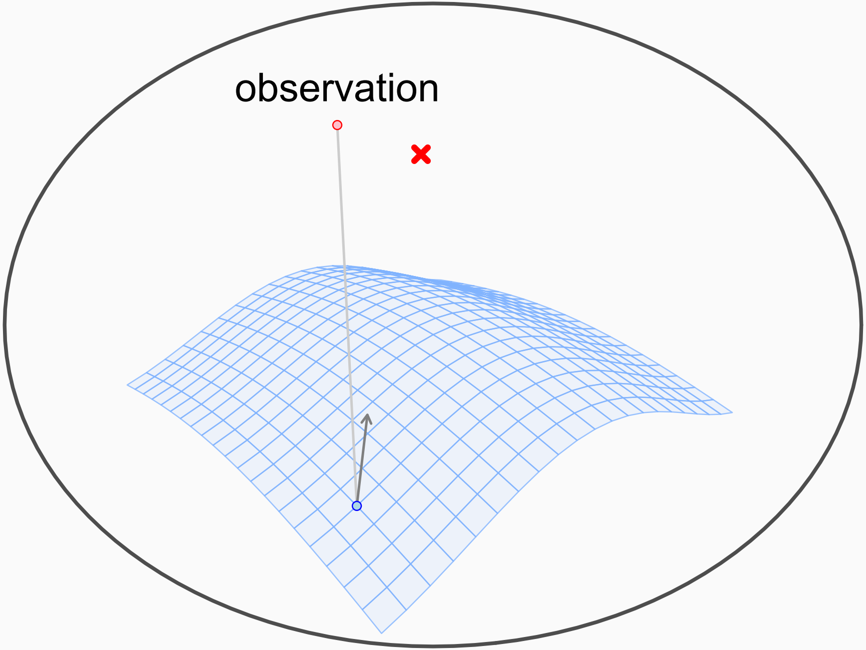
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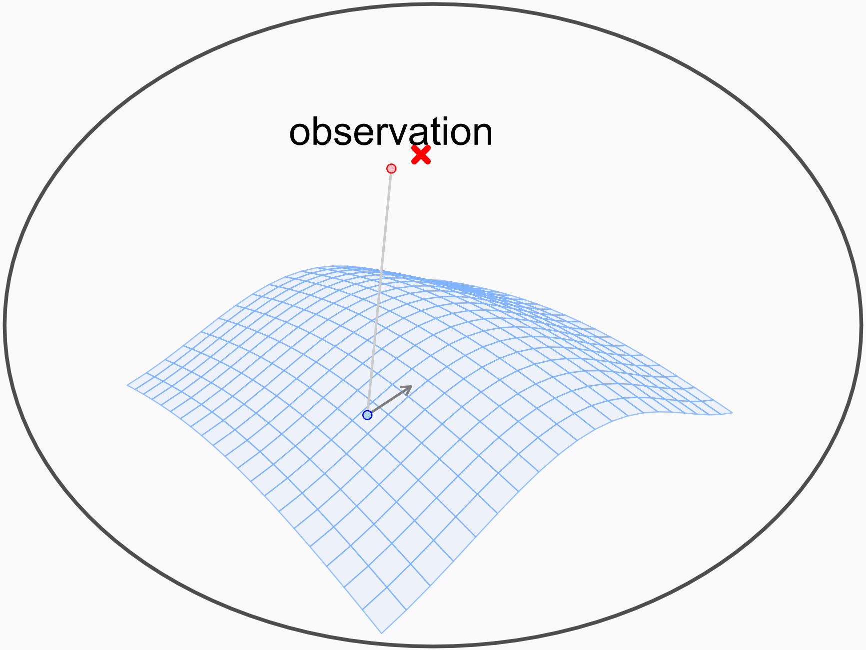
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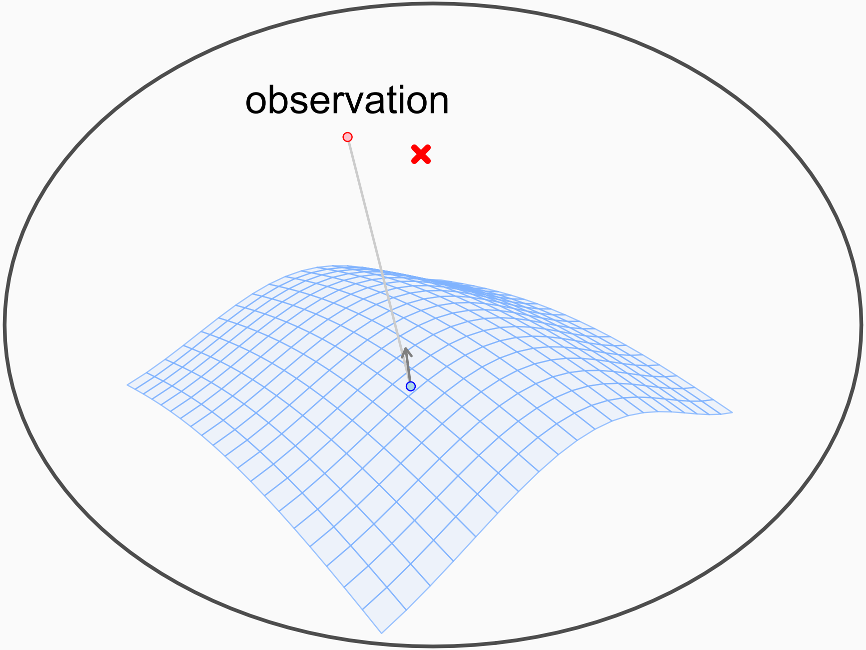
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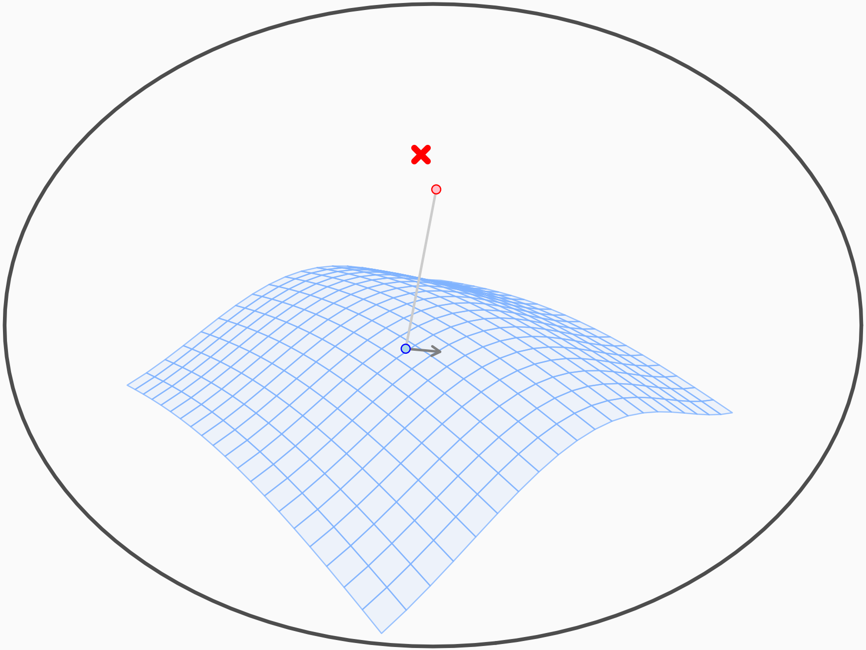
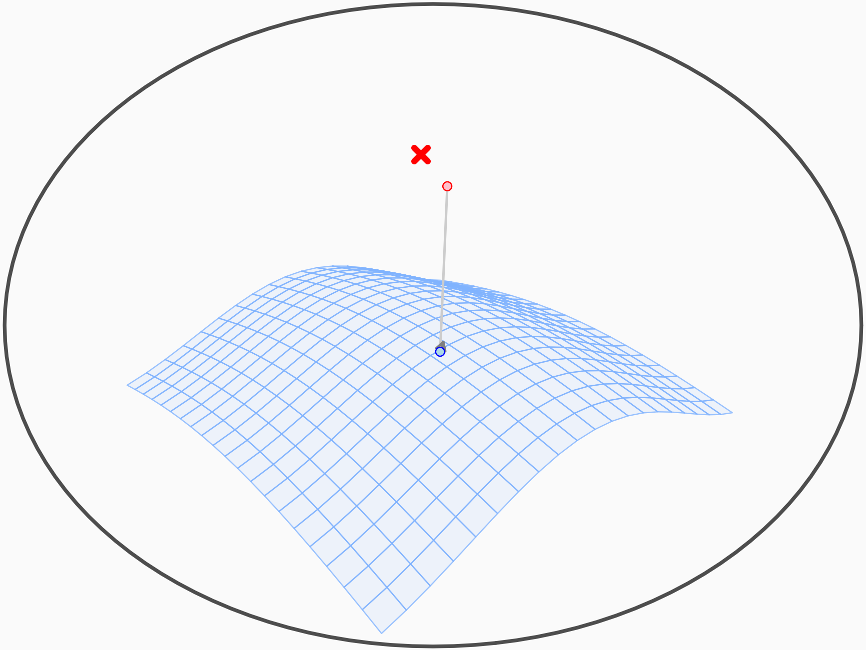
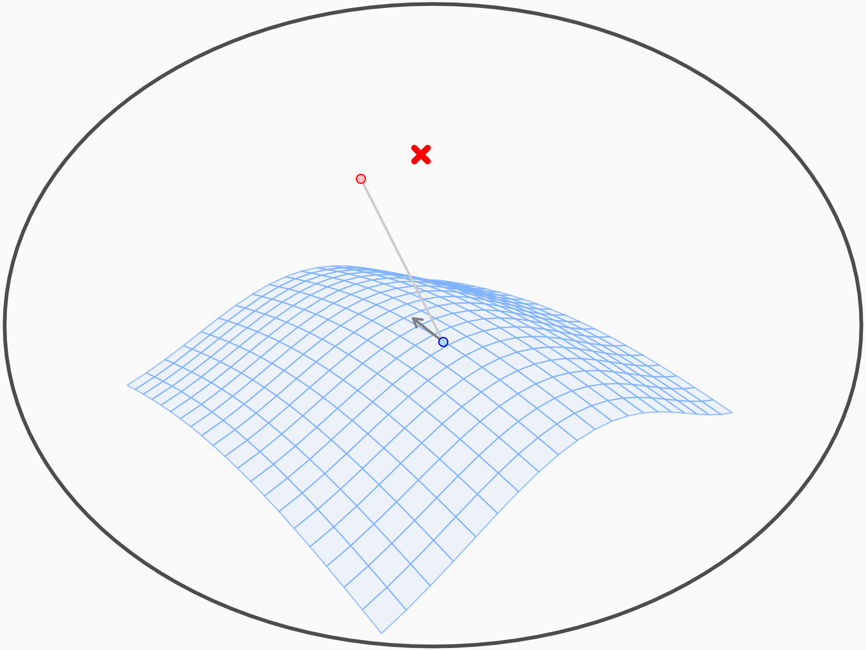
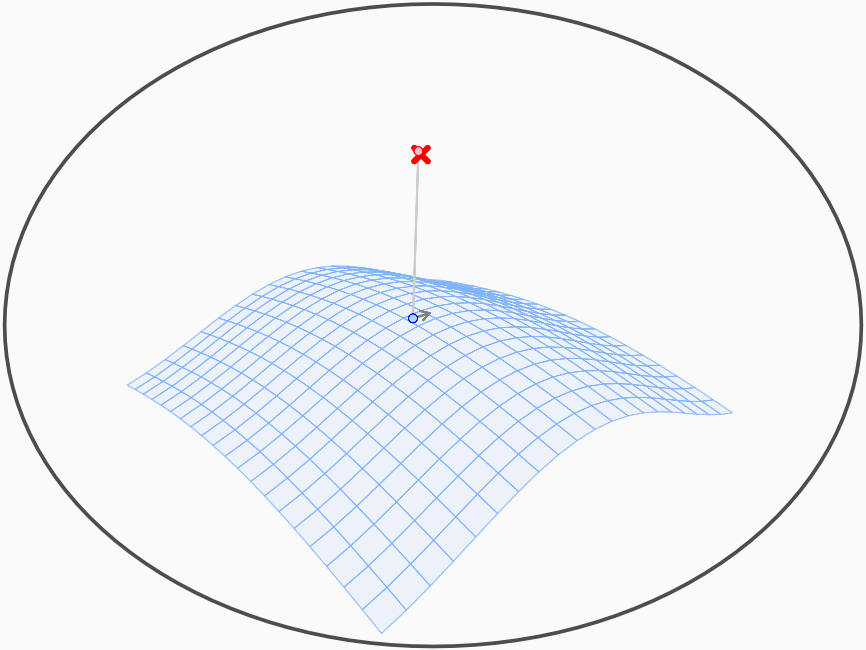
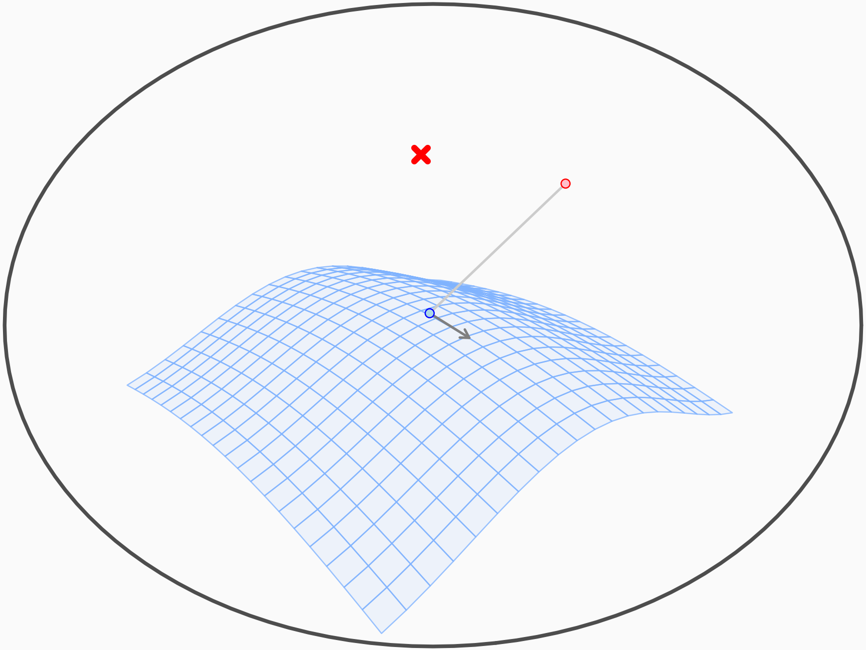
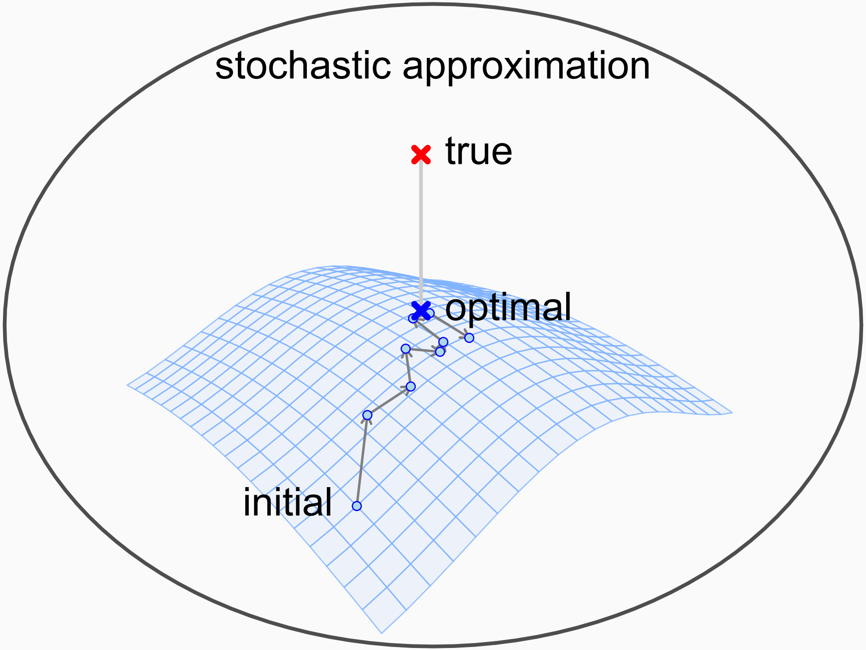











stochastic approximation
true
optimal
initial

- is on-line learning inferior to batch?
- how on-line estimators behave?
- what are good learning parameters?

Problem Formulation

Lemma (Godambe, 1991)

The distribution of $\hat{\theta}_t$ converges to the normal distribution

$$\hat{\theta}_t \sim \mathcal{N}\left(\theta_*, \frac{1}{t}V\right), \quad V = H^{-1}GH^{-1}$$

under some regularity condition, where

$$G = \mathbb{E}_{Z\sim P}\left[\nabla l(Z;\theta)\nabla l(Z;\theta)^\top\right],$$
$$H = \mathbb{E}_{Z\sim P}\left[\nabla\nabla l(Z;\theta)\right],$$

and θ is the optimal parameter of the population loss:

$$\theta = \arg\min_\theta L(\theta).$$

Theorem

The expectation of the population loss is asymptotically given by

$$\mathbb{E}\left[L(\hat{\theta}_t)\right] = L(\theta_*) + \frac{1}{2t}\operatorname{tr} GH^{-1} + o\left(\frac{1}{t}\right),$$

where the expectation is taken with respect to D_t.

The variance is asymptotically given by

$$\mathbb{V}\left[L(\hat{\theta}_t)\right] = \frac{1}{2t^2}\operatorname{tr} GH^{-1}GH^{-1} + o\left(\frac{1}{t^2}\right).$$

Theorem

The expectation of the empirical loss is asymptotically given by

$$\mathbb{E}\left[\hat{L}_t(\hat{\theta}_t)\right] = L(\theta) - \frac{1}{2t}\operatorname{tr} GH^{-1} + o\left(\frac{1}{t}\right),$$

where the expectation is taken with respect to D_t.

The variance is asymptotically given by

$$\mathbb{V}\left[\hat{L}_t(\hat{\theta}_t)\right] = \frac{1}{t}\mathbb{V}_{Z\sim P}\left[l(Z;\theta)\right] + o\left(\frac{1}{t}\right).$$

- generalization error:

$$\mathbb{E}\left[L(\hat{\theta}_t)\right] = L(\theta_*) + \frac{1}{2t}\operatorname{tr} GH^{-1} + o\left(\frac{1}{t}\right),$$

- training error:

$$\mathbb{E}\left[\hat{L}_t(\hat{\theta}_t)\right] = L(\theta) - \frac{1}{2t}\operatorname{tr} GH^{-1} + o\left(\frac{1}{t}\right),$$

Corollary (Akaike, 1974)

The generalization error is estimated from the training error by correcting the bias as

$$L(\hat{\theta}_t) = \hat{L}_t(\hat{\theta}_t) + \frac{1}{t}\operatorname{tr} GH^{-1}.$$

In the case of the maximum likelihood estimation, if the ground truth is realized by θ,

$$L(\hat{\theta}_t) = \hat{L}_t(\hat{\theta}_t) + \frac{m}{t} \quad (m: \text{ dim. of } \theta),$$

because $H = G$.

Lemma (Akahira & Takeuchi, 1981; Bottou & Le Cun, 2005)

Let $\hat{\theta}_{t-1}$ and $\hat{\theta}_t$ be estimates for D_{t-1} and $D_t = D_{t-1} \cup \{z_t\}$. Then

$$\hat{\theta}_t = \hat{\theta}_{t-1} - \frac{1}{t}\hat{H}_t^{-1}\nabla l(z_t; \hat{\theta}_{t-1}) + \mathcal{O}_p\left(\frac{1}{t^2}\right)$$

holds under some mild condition, where $\hat{H}_t$ is the empirical Hessian defined by

$$\hat{H}_t = \frac{1}{t}\sum_{z_i \in D_t} \nabla\nabla l(z_i; \hat{\theta}_{t-1}).$$

- batch learning:

$$\hat{\theta}_t = \hat{\theta}_{t-1} - \frac{1}{t}\hat{H}_t^{-1}\nabla l(z_t; \hat{\theta}_{t-1}) + \text{(higher order term)}$$

- optimal on-line learning:

$$\theta_t = \theta_{t-1} - \frac{1}{t}\tilde{H}_{t-1}^{-1}\nabla l(z_t; \theta_{t-1}) + \text{(higher order term)}$$

- optimal design: Newton-Raphson $+ 1/t$-annealing

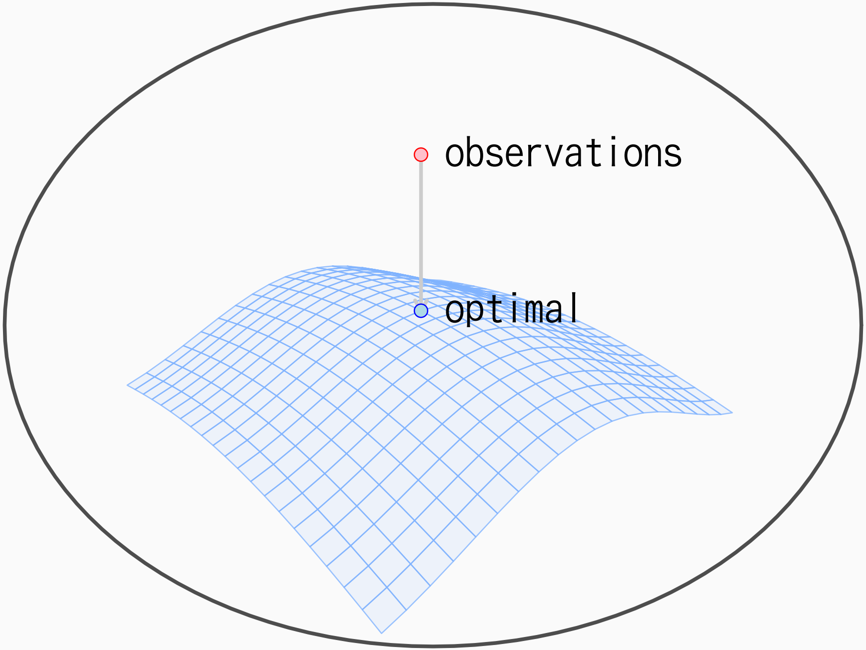
$$\Phi_t = \frac{1}{t}\hat{H}_t^{-1},$$

- on-line estimate of Hessian: %(Kalman filtering;Bottou, 1998) (MLE case; Bottou, 1998)

$$\Phi_{t+1} = \Phi_t - \frac{\Phi_t \nabla l \nabla l^{\mathsf{T}} \Phi_t}{1 + \nabla l^{\mathsf{T}} \Phi_t \nabla l}$$
$$\text{where } \nabla l = \nabla l(z_{t+1}; \theta_t)$$

  stochastic-BFGS (Nocedal et al, 2014), etc.

- rate of convergence: equivalent with batch learning (NM, 1998; NM & Amari, 1999; Bottou & Le Cun, 2005)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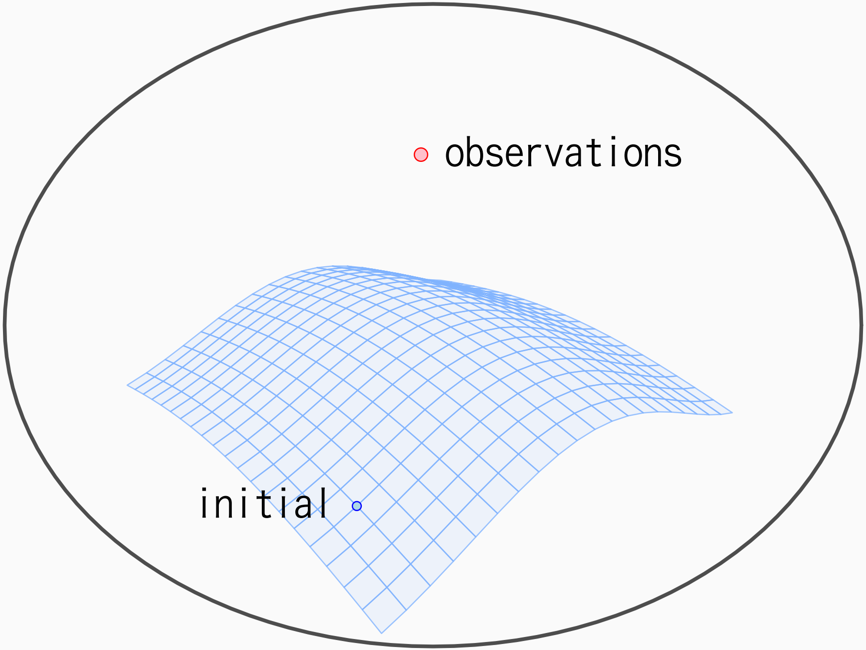
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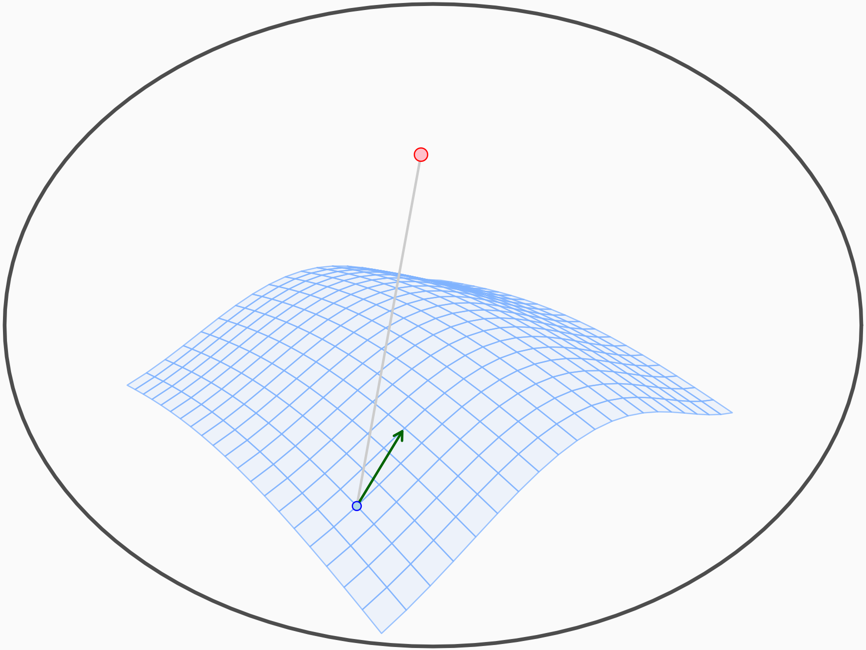
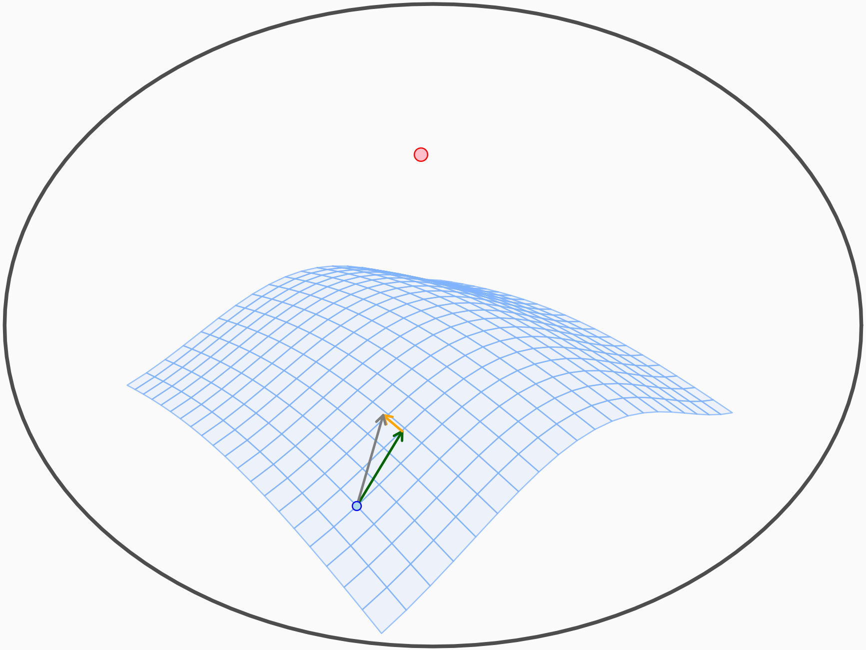
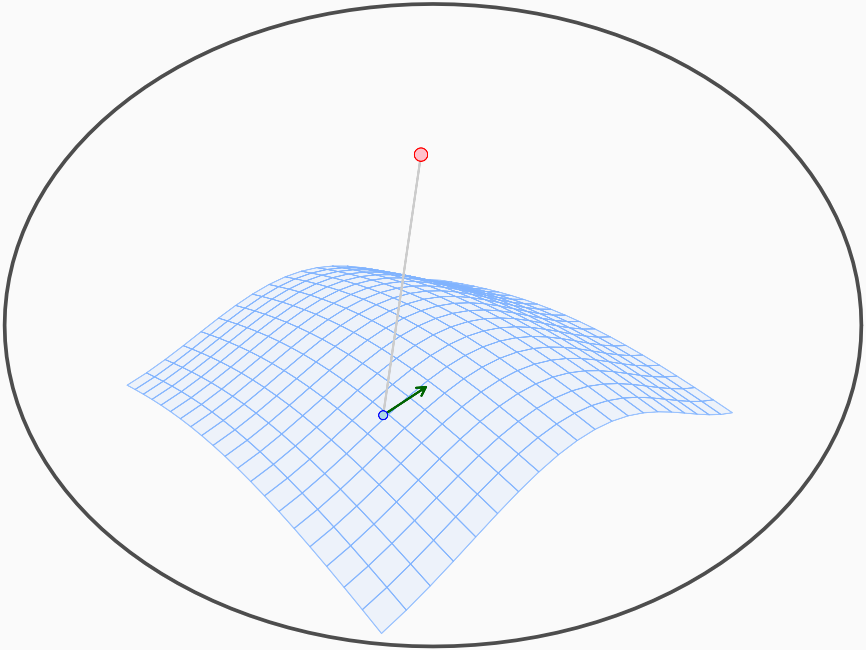
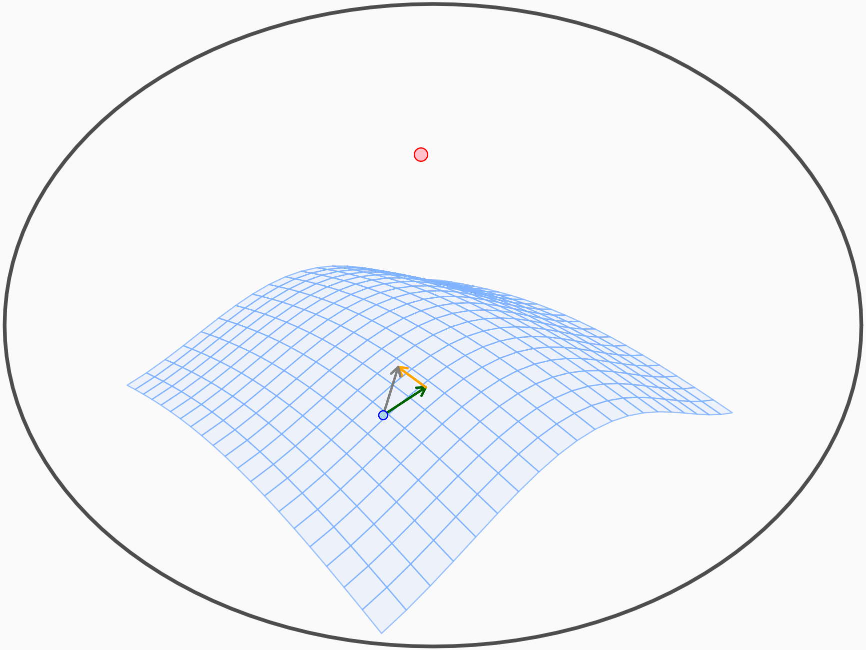
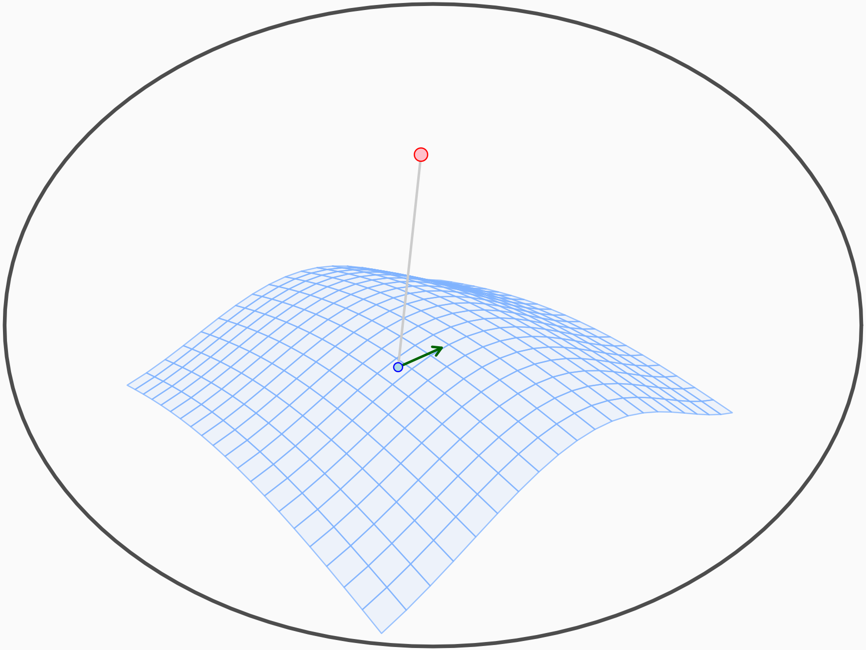
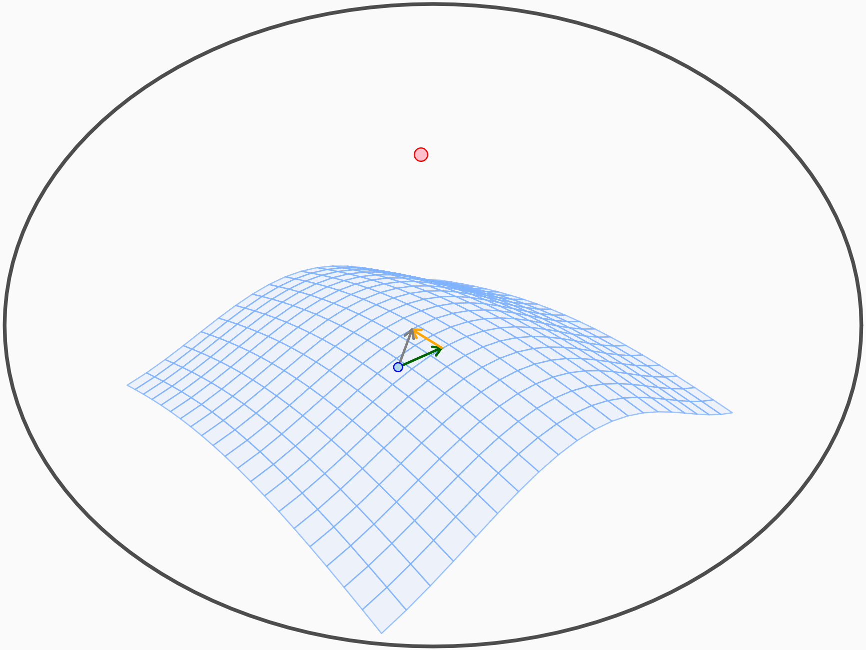


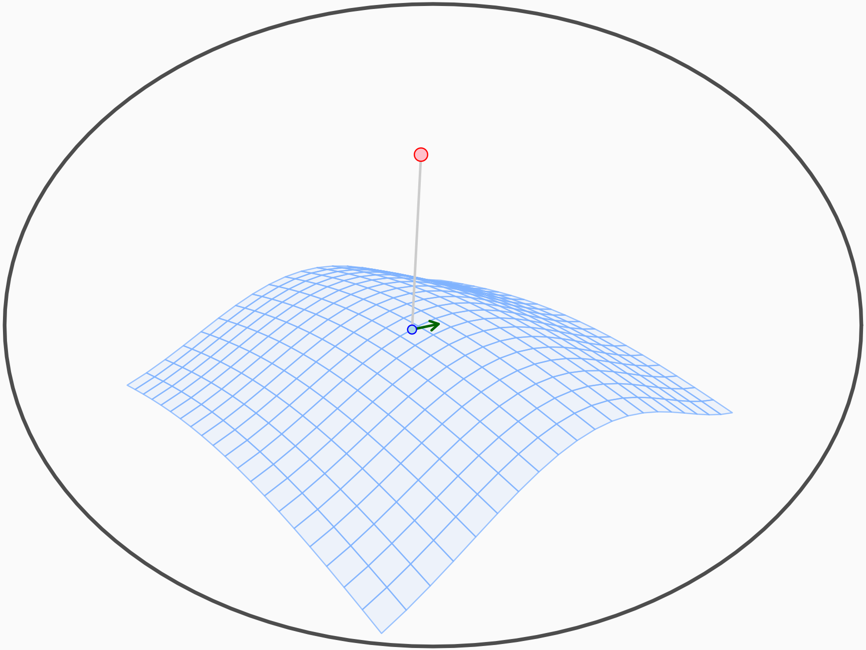


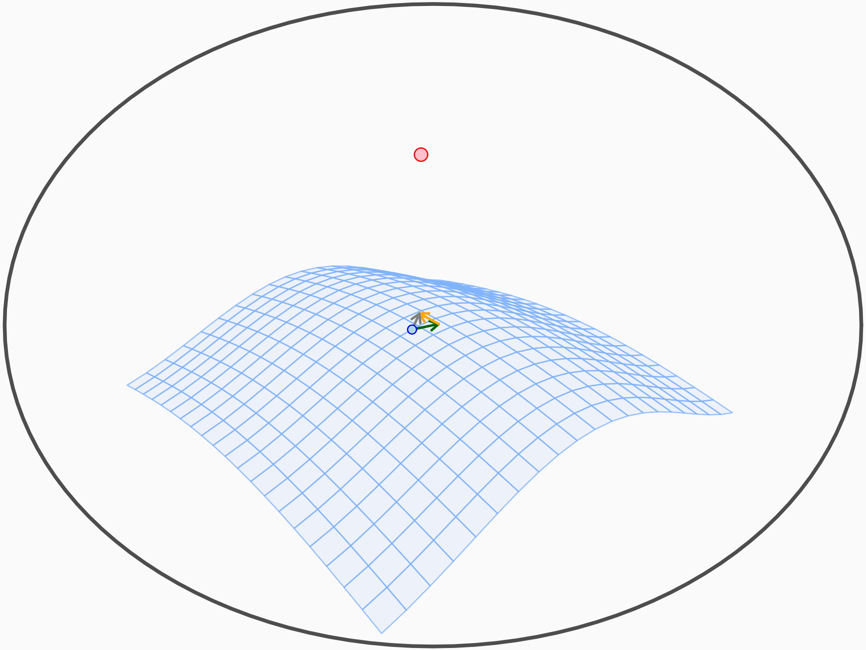


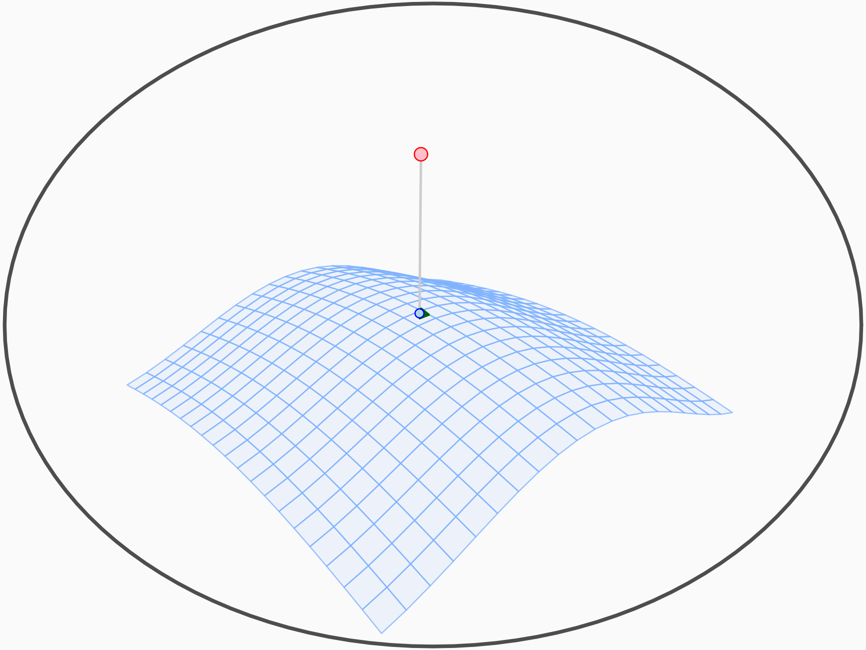


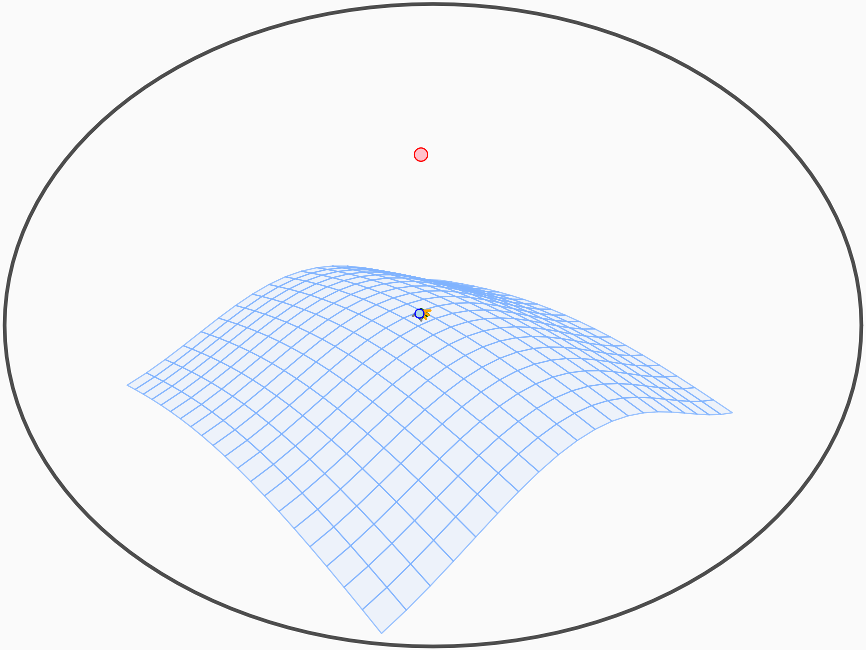


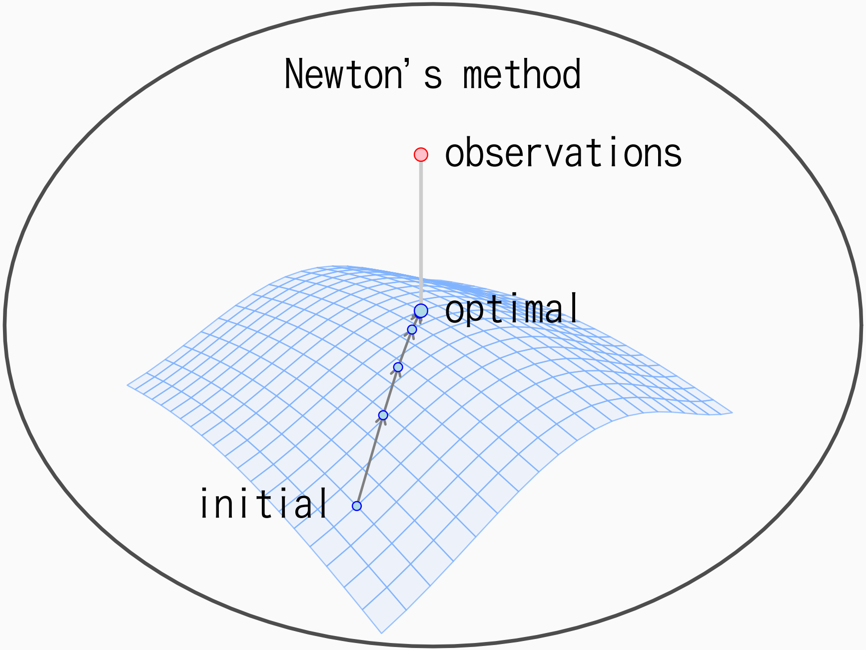











Newton's method
observations
optimal
initial

Lemma (Amari, 1967)

$$\mathbb{E}^{\theta_{t+1}}\left[f(\theta_{t+1})\right] = \mathbb{E}^{\theta_t}\left[f(\theta_t)\right] - \mathbb{E}^{\theta_t}\left[\nabla f(\theta_t)^\top \Phi_t \nabla L(\theta_t)\right] + \frac{1}{2}\operatorname{tr}\mathbb{E}^{\theta_t}\left[\Phi_t G(\theta_t)\Phi_t^\top \nabla\nabla f(\theta_t)\right] + \mathcal{O}(\|\Phi_t\|^3)$$

holds for any smooth function $f(\theta)$, where $\mathbb{E}^{\theta}$ denotes the expectation with respect to θ, and $G(\theta)$ is defined by

$$G(\theta) = \mathbb{E}_{Z\sim P}\left[\nabla l(Z;\theta)\nabla l(Z;\theta)^\top\right].$$

Definition

Let A be an $m \times m$ square matrix and M be an $m \times m$ symmetric matrix. We define two linear operators as follows:

$$\Xi_A M = AM + (AM)^\top,$$
$$\Omega_A M = AMA^\top.$$

Lemma

Around the optimal parameter, the following approximated recursive relations for the expectation $\bar{\theta}_t = \mathbb{E}^{\theta_t}[\theta_t]$ and the covariance $V_t = \mathbb{V}^{\theta_t}[\theta_t]$ hold:

$$\bar{\theta}_{t+1} = \bar{\theta}_t - Q_t(\bar{\theta}_t - \theta),$$
$$V_{t+1} = V_t - \Xi_{Q_t} V_t + \Omega_{Q_t} V - \Omega_{Q_t}(\bar{\theta}_t - \theta)(\bar{\theta}_t - \theta)^\top,$$

where

$$Q_t = \Phi_t H, \quad V = H^{-1} G H^{-1}.$$

(note: $\Xi_A M = AM + (AM)^\top$, $\Omega_A M = AMA^\top$)

Theorem

Let Φ be C/t, where C is a constant matrix. If $\lambda_{\min}(CH) \geq 1$, the leading terms are given by

$$\bar{\theta}_t = \theta + S_t(\theta_0 - \theta), \quad S_t = \prod_{\tau=2}^{t} \left(I - \frac{CH}{\tau} \right) = \mathcal{O}\left(\frac{1}{t^{\lambda_{\min}}} \right),$$

$$V_t = \left[\left(\Xi_{CH} - I \right)^{-1} \Omega_{CH} \right] \frac{1}{t} V, \quad V = H^{-1} G H^{-1},$$

where θ_0 is an initial parameter.

Lemma

Let $\lambda_i,\ i = 1, \ldots, m$ be eigenvalues of A. The eigenvalues of Ξ_A and Ω_A are given by

$$
\begin{aligned}
\Xi_A &: \lambda_i + \lambda_j,\ \ i, j = 1, \ldots, m, \\
\Omega_A &: \lambda_i \lambda_j,\ \ i, j = 1, \ldots, m.
\end{aligned}
$$

.

This follows by the relation

$$\mathrm{cs}(ABC) = (C^{\top} \otimes A)\mathrm{cs}B$$

for any $m \times m$ square matrices A, B, C. $\square$

- larger $\lambda_{\min}$ is advantageous to faster convergence of $\bar{\theta}_t$.
- $(\Xi_{CH} - I)^{-1}\Omega_{CH}$ expands V/t, which is the minimum covariance attained by batch learning.
- eigenvalues of $(\Xi_{CH} - I)^{-1}\Omega_{CH}$ are given by

  $$\frac{\lambda_i \lambda_j}{\lambda_i + \lambda_j - 1},$$

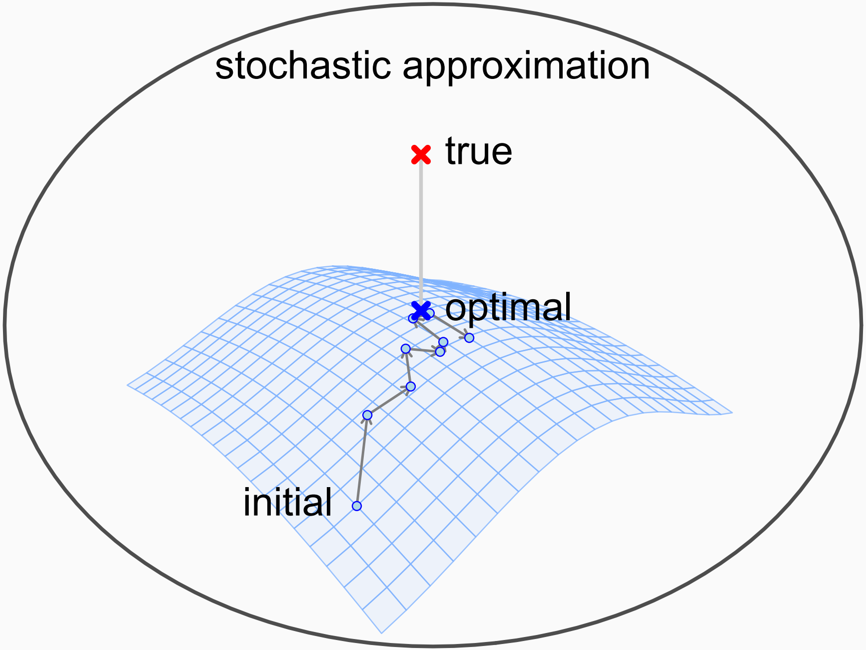
  where λ_i's are eigenvalues of CH.
- if $C = H^{-1}$, %i.e. $CH = I$, all the eigenvalues of $(\Xi_I - I)^{-1}\Omega_I$ are equal to 1, i.e. $V_t = V/t$.
- $\Phi_t = H^{-1}/t$ is optimal.

- on-line learning:

$$\mathbb{E}\left[(\theta_t - \theta)(\theta_t - \theta)^\top\right] = \mathbb{V}\left[\theta_t\right] + \mathbb{E}\left[\theta_t - \theta\right]\mathbb{E}\left[\theta_t - \theta\right]^\top$$
$$= \frac{1}{t}V + \mathcal{O}\left(\frac{1}{t^2}\right).$$

- batch learning:

$$\mathbb{E}\left[(\hat{\theta}_t - \theta)(\hat{\theta}_t - \theta)^\top\right] = \frac{1}{t}V + \mathcal{O}\left(\frac{1}{t^2}\right).$$


stochastic approximation
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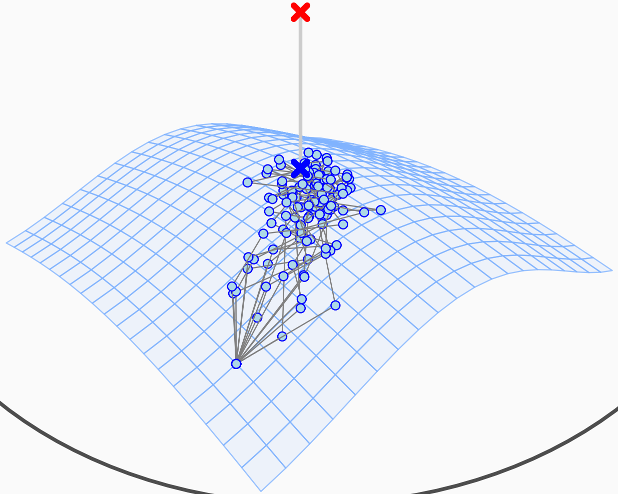
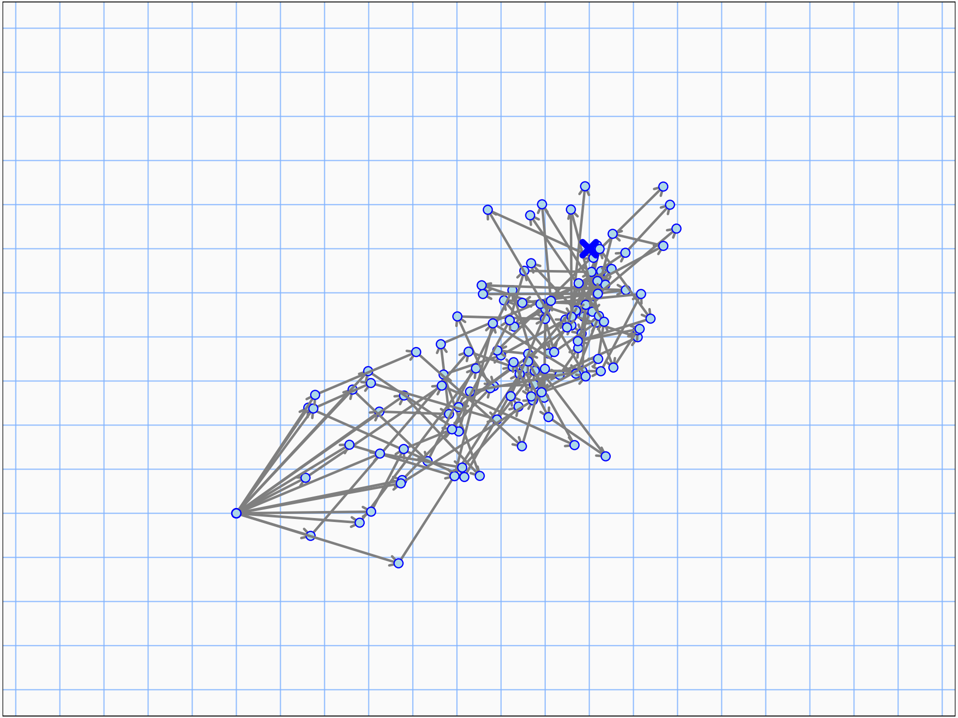
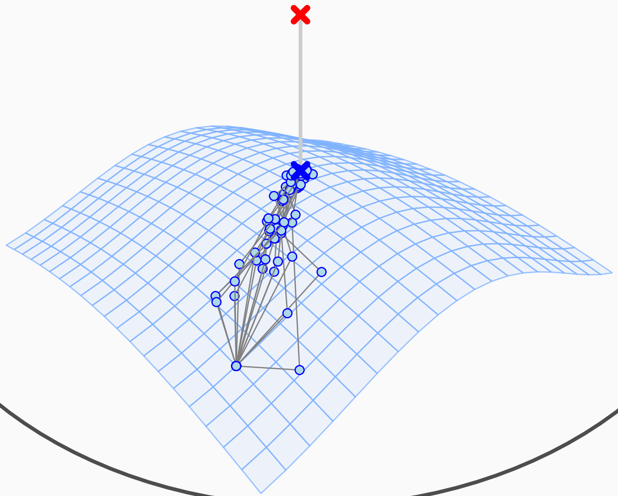
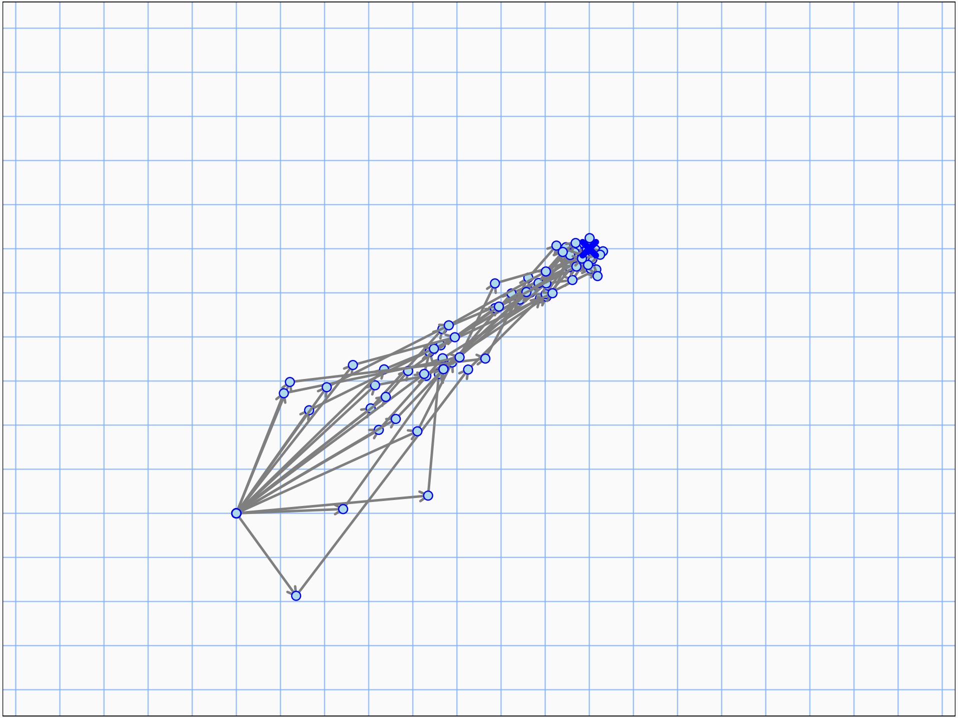
fixed learning rate





optimal learning rate





Illustrative Example

a method for evaluating the relative skill levels of players

- Elo rating: Arpad Elo, 1960
  used in competitor-versus-competitor games such as chess
  scores given to players are updated according to game results
- Glicko rating: Mark Glickman, 1997
  including confidence of estimated skill levels
- TrueSkill: Ralf Herbrich et al., 2007
  extension to multiplayer games
  skill levels are random variables (Bayesian framework)

- score: $\theta = (\theta^1, \theta^2, \dots)$
- event: $z_t = (a \succ b)$ (player a beats player b at time t)
- probability model:

$$\Pr(a \succ b) = P(z_t; \theta) = \frac{1}{1 + \exp(\gamma \cdot (\theta^b - \theta^a))},$$

  where γ is defined such that a player whose rating is 200 points greater than the other is expected to have a 75\
- loss function: (negative log loss)

$$l(z_t; \theta) = -\log P(z_t; \theta) = \log(1 + \exp(\gamma \cdot (\theta^b - \theta^a)))$$

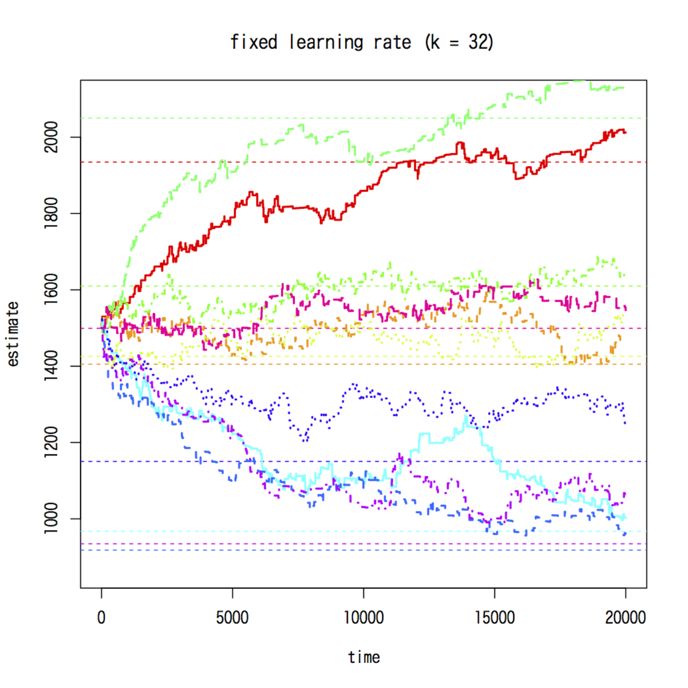
- gradient:

$$\frac{\partial}{\partial \theta^i} l(z_t;\theta) = \begin{cases} 0, & i \neq a, b \\ -\gamma \cdot (1 - P(z_t;\theta)), & i = a \text{ (winner)} \\ +\gamma \cdot (1 - P(z_t;\theta)), & i = b \text{ (looser)} \end{cases}$$

- update rule:

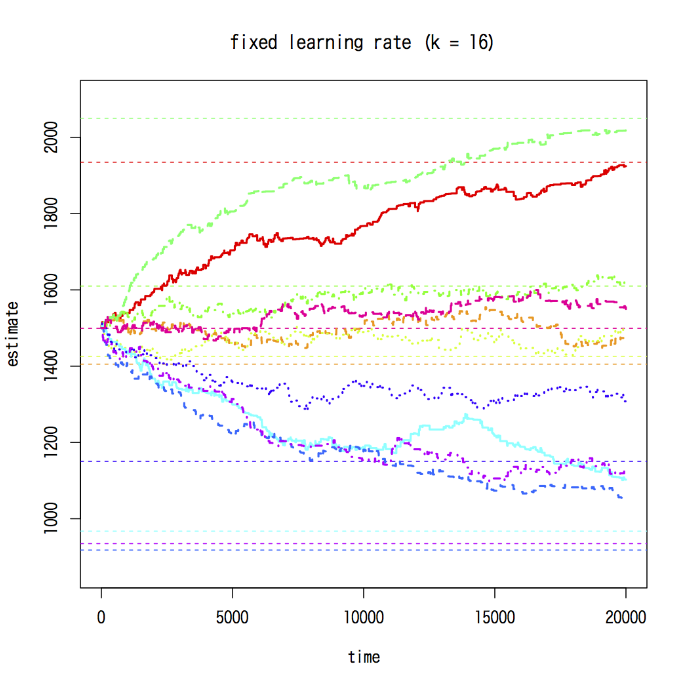
$$\begin{aligned} \theta_{t+1} &= \theta_t - \varepsilon \nabla l(z_t;\theta) \\ &= \theta_t + (0, \dots, \underbrace{\varepsilon\gamma(1-P)}_{a}, \dots, \underbrace{-\varepsilon\gamma(1-P)}_{b}, \dots, 0)^T \end{aligned}$$

where $k = \varepsilon\gamma =$ 32 for novices, 16 for professionals.



fixed rate\ $\Phi_t = \varepsilon I$

- 10 players out of 100
- 20000 games $\{(400[\text{games}/\text{pl.}])\}$
- $k = 32, 16, 64$
- $\theta_0^i = 1500$



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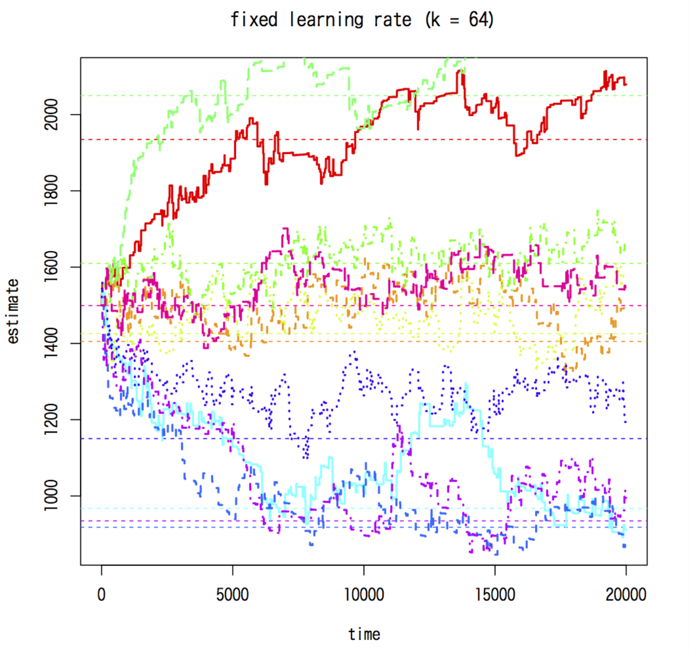


fixed rate\ $\Phi_t = \varepsilon I$

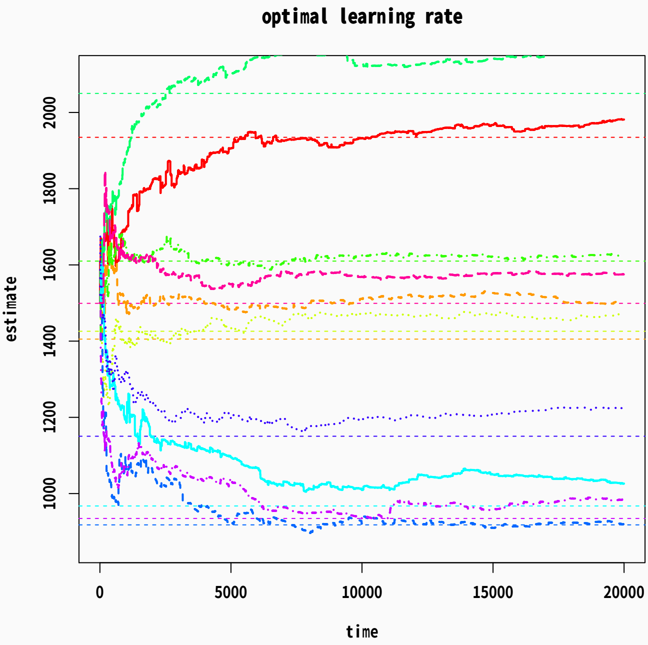
- 10 players out of 100
- 20000 games {(400[games/pl.])}
- $k = 32, 16, 64$
- $\theta_0^i = 1500$

- update rule: (Φ: matrix)

$$
\begin{aligned}
\theta_{t+1} &= \theta_t - \Phi_t \nabla l(z_t; \theta_t), \\
\Phi_{t+1} &= \Phi_t - \frac{\Phi_t \nabla l_t \nabla l_t^{\mathsf{T}} \Phi_t}{1 + \nabla l_t^{\mathsf{T}} \Phi_t \nabla l_t}, \\
\nabla l_t &= \nabla l(z_{t+1}; \theta_t) \\
&= (0, \ldots, \underbrace{\gamma(1-P)}_{a}, \ldots, \underbrace{-\gamma(1-P)}_{b}, \ldots, 0)^T
\end{aligned}
$$

- initial value:

$$\Phi_0 = kI \quad I \text{ is the identity matrix}$$



optimal rate

- 10 players
  out of 100
- 20000 games
  $\{(400[\text{games/pl.}])\}$
- sensitive to initial value

- original update rule: $\Delta\theta = -\varepsilon \nabla l(z_t; \theta)$
  - only related players are updated: $\Delta\theta^i = 0,\ i \neq a, b$.
  - sum of θ is kept constant: $\mathbf{1}^\intercal \Delta\theta = 0$.
- optimal update rule: $\Delta\theta = -\Phi_t \nabla l(z_t; \theta)$
  - all the players are updated, because $\Phi_t = \hat{H}_t^{-1}/t$ is a dense matrix.
  - sum of θ is not necessarily kept constant.
- our problem: design Φ_t to fit the original restriction.

- 1 vs 1 case: (players a and b)

$$\Delta\theta = \alpha \boldsymbol{a}, \quad \boldsymbol{a}^\top = \begin{array}{c} \begin{array}{cccc} a & b & c & \end{array} \\ \begin{pmatrix} 1 & -1 & 0 & \cdots \end{pmatrix} \end{array},$$

or

$$B^\top \Delta\theta = 0, \quad B^\top = \begin{array}{c} \begin{array}{ccccc} a & b & c & d & \end{array} \\ \begin{pmatrix} 1 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ \vdots & \vdots & & & \ddots \end{pmatrix} \end{array}.$$

- 2 vs 2 case: (players a+b and c+d)

$$\Delta\theta = A\alpha, \quad A^\top = \begin{array}{c} \begin{array}{cccccc} a & b & c & d & e & \end{array} \\ \begin{pmatrix} 1 & 0 & -1 & 0 & 0 & \cdots \\ 1 & 0 & 0 & -1 & 0 & \cdots \\ 0 & 1 & -1 & 0 & 0 & \cdots \end{pmatrix} \end{array},$$

or

$$B^\top \Delta\theta = 0, \quad B^\top = \begin{array}{c} \begin{array}{ccccccc} a & b & c & d & e & f & \end{array} \\ \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 1 & \cdots \\ \vdots & \vdots & & & & & \ddots \end{pmatrix} \end{array}.$$

Problem A

Find an "optimal" gradient $\Delta\theta = \Phi\nabla l(z;\theta)$ subject to

$$\Delta\theta \in \operatorname{Im} A, \quad (\Delta\theta = A\alpha,\ \alpha \in \mathbb{R}^k)$$

for a matrix $A \in \mathbb{R}^{m\times k}$.

Problem B

Find an "optimal" gradient $\Delta\theta = \Phi\nabla l(z;\theta)$ subject to

$$\Delta\theta \in \operatorname{Ker} B^\top, \quad (B^\top\Delta\theta = 0)$$

for a matrix $B \in \mathbb{R}^{m\times(m-k)}$,

cf. $f(\theta) = \text{const.} \Rightarrow \nabla f(\theta)^\top\Delta\theta = 0$

- optimality is defined in terms of

$$\text{minimize } \|H^{-1}\nabla l - \Delta\theta\|_M,$$

where $\|x\|_M^2 = \langle x, x\rangle_M$ and $\langle x, y\rangle_M = \langle Mx, y\rangle$.
- M is chosen as H, because
  - quadratic approximation of population loss:

$$\|\theta - \theta\|_H^2 = (\theta - \theta)^\top H(\theta - \theta) = L(\theta) - L(\theta)$$

  - Mahalanobis distance in maximum likelihood case:

$$\mathbb{V}[\hat{\theta}_t] = \frac{1}{t}H^{-1}GH^{-1} = \frac{1}{t}H^{-1}$$

% - (Φ_t becomes symmetric.)

- decompose Φ_t into scalar and matrix parts as

$$\Phi_t = \varepsilon_t C, \quad (\text{e.g., } \varepsilon_t = 1/t)$$

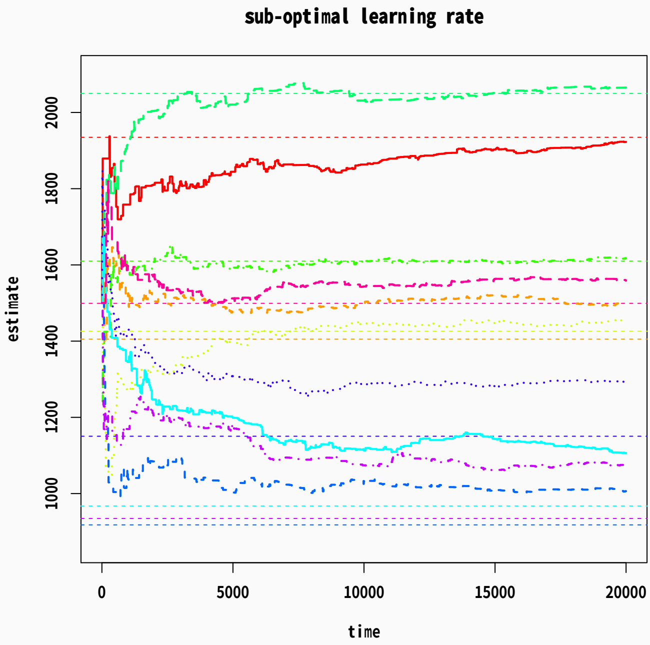
- solutions for the problems are:

Problem A

$$C_A = A(A^\top HA)^{-1}A^\top$$

Problem B

$$C_B = H^{-1} - H^{-1}B(B^\top H^{-1}B)^{-1}B^\top H^{-1}$$



sub-optimal rate

- 10 players out of 100
- 20000 games {(400[games/pl.])}

- C_A and C_B are symmetric (only when $M = H$).
- $C_A H$ or $C_B H$ is a projection matrix:

$$\lambda = \begin{cases} 1, & v \in \operatorname{Im} A \text{ or } \operatorname{Ker} B, \\ 0, & \text{otherwise.} \end{cases}$$

- if k is small, calculating C_A is more efficient than C_B.
- only a few parameters are updated, however convergence is as good as optimal case.
  (information loss is quite small in some case)

Conclusion

we have investigated

- dynamics of convergence phase of on-line learning,
- conditions for optimal convergence rate,
- optimal projection of gradients to subspaces,

practical applications would be

- skill level rating systems,
- on-line learning for Bradley-Terry model,
- distributed control systems.

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