Hyper-parameters Selection by Automatic Differentiation

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Joint works with

       

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Parametric estimators

Estimator

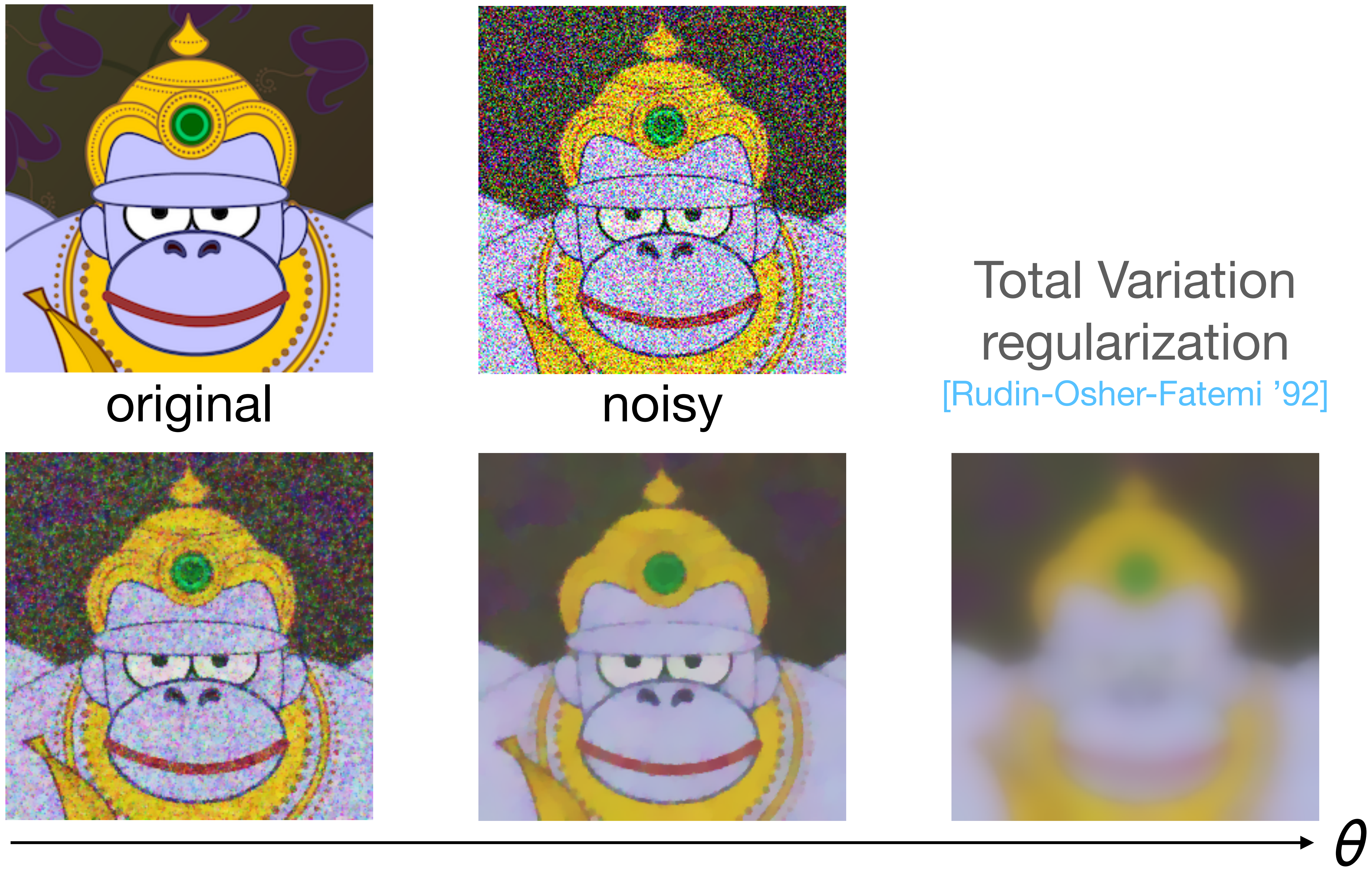
$$\hat{w}_\theta : \begin{cases} \mathbb{R}^n & \longrightarrow \mathbb{R}^p \\ y & \longmapsto \hat{w}_\theta(y) \end{cases}$$

observations

Hyper-parameters

$$\theta \in \Theta \subseteq \mathbb{R}^l$$

parameter space



Typical example

linear regression

$$y = X w_{\text{true}} + \varepsilon$$

design matrix, ground truth, noise

regularization *a.k.a* variational methods

$$\hat{w}_\theta(y) \in \operatorname{argmin}_w \text{datafit}(w, y) + \text{regularity}(w, \theta)$$

trade-off

e.g. Lasso: $\operatorname{argmin}_w \|y - Xw\|_2^2 + \theta \|w\|_1$ [Chen-Donoho '94, Tibshirani '95]

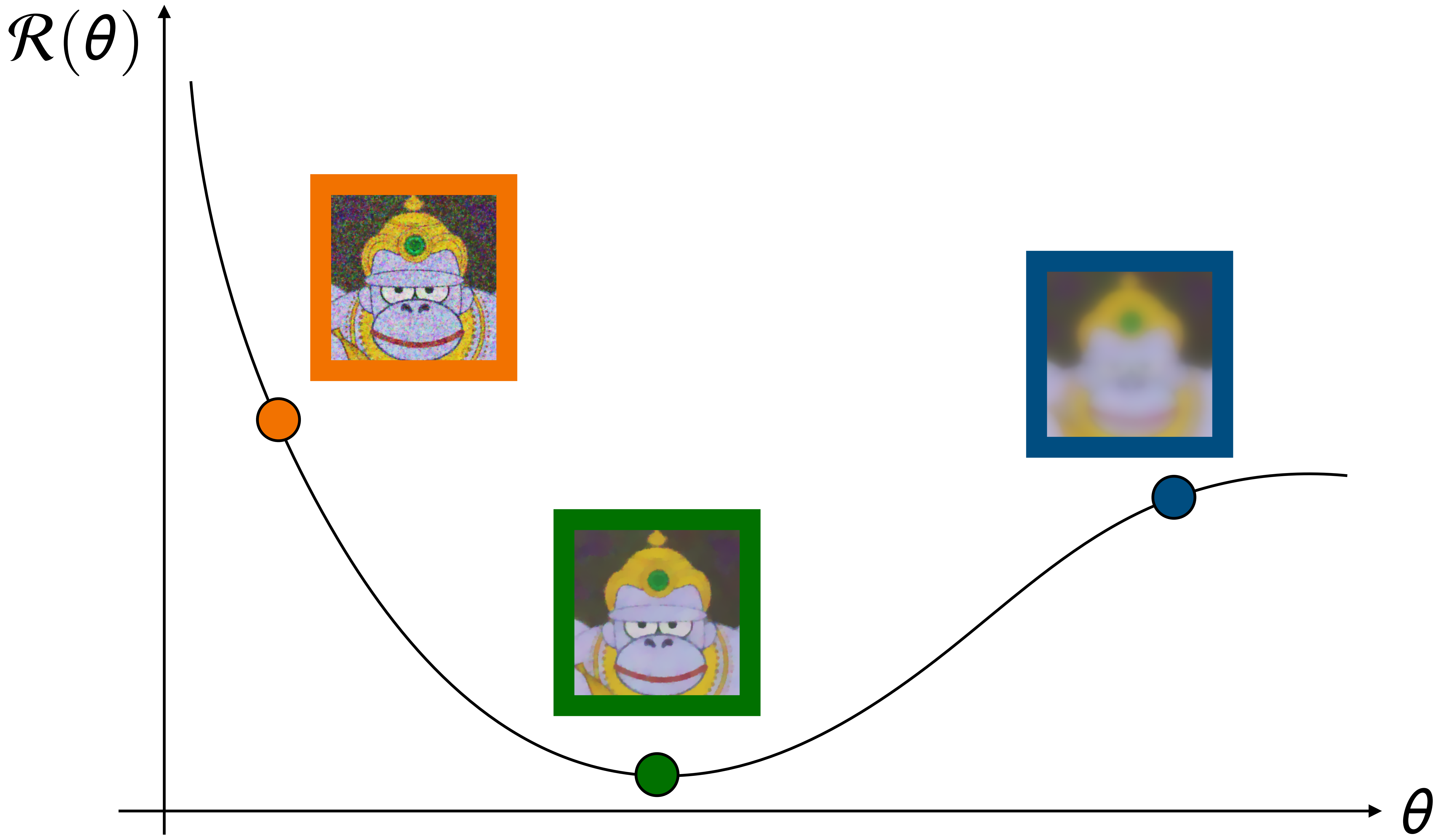
Selection criteria

Estimator

$\hat{w}_\theta : \mathbb{R}^n \longrightarrow \mathbb{R}^p$ estimator

$\theta \in \Theta$ hyper-parameter

$\mathcal{R} : \Theta \longrightarrow \mathbb{R}$ criterion



Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}}\ \mathcal{R}(\theta)$

(or close to it)

Inverse problems

$y = X w_{\text{true}} + \varepsilon$

estimation risk

[Rice '86]

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\| \hat{w}_\theta(y) - w_{\text{true}} \|_2^2 \right)$$

Machine learning

validation set: $y^{\text{val}}, X^{\text{val}}$

hold-out loss

[Stone-Ramer '65]

$$\mathcal{R}(\theta) = \| y^{\text{val}} - X^{\text{val}} \hat{w}_\theta(y) \|_2^2$$

projected risk
cross-validation
model criteria
...

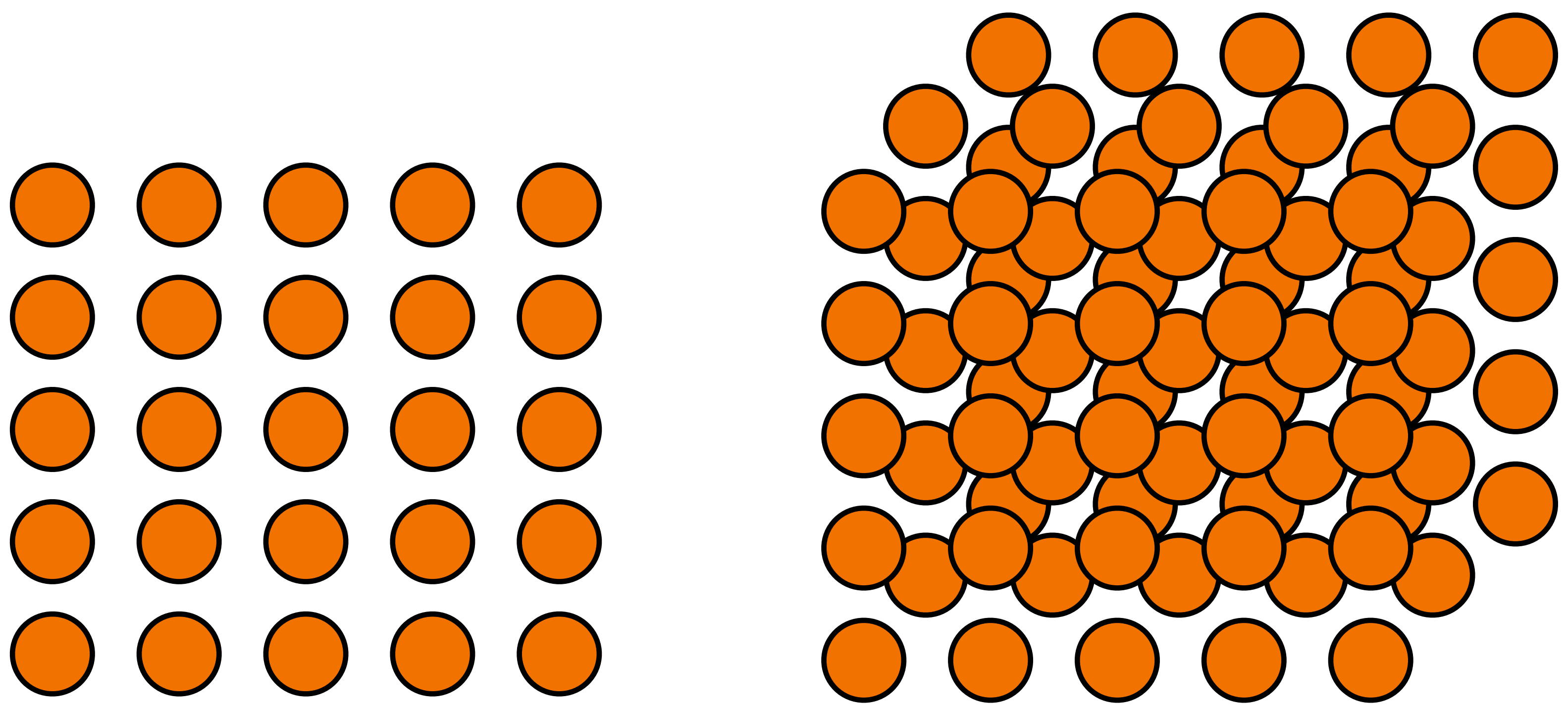
Grid search

Algorithm

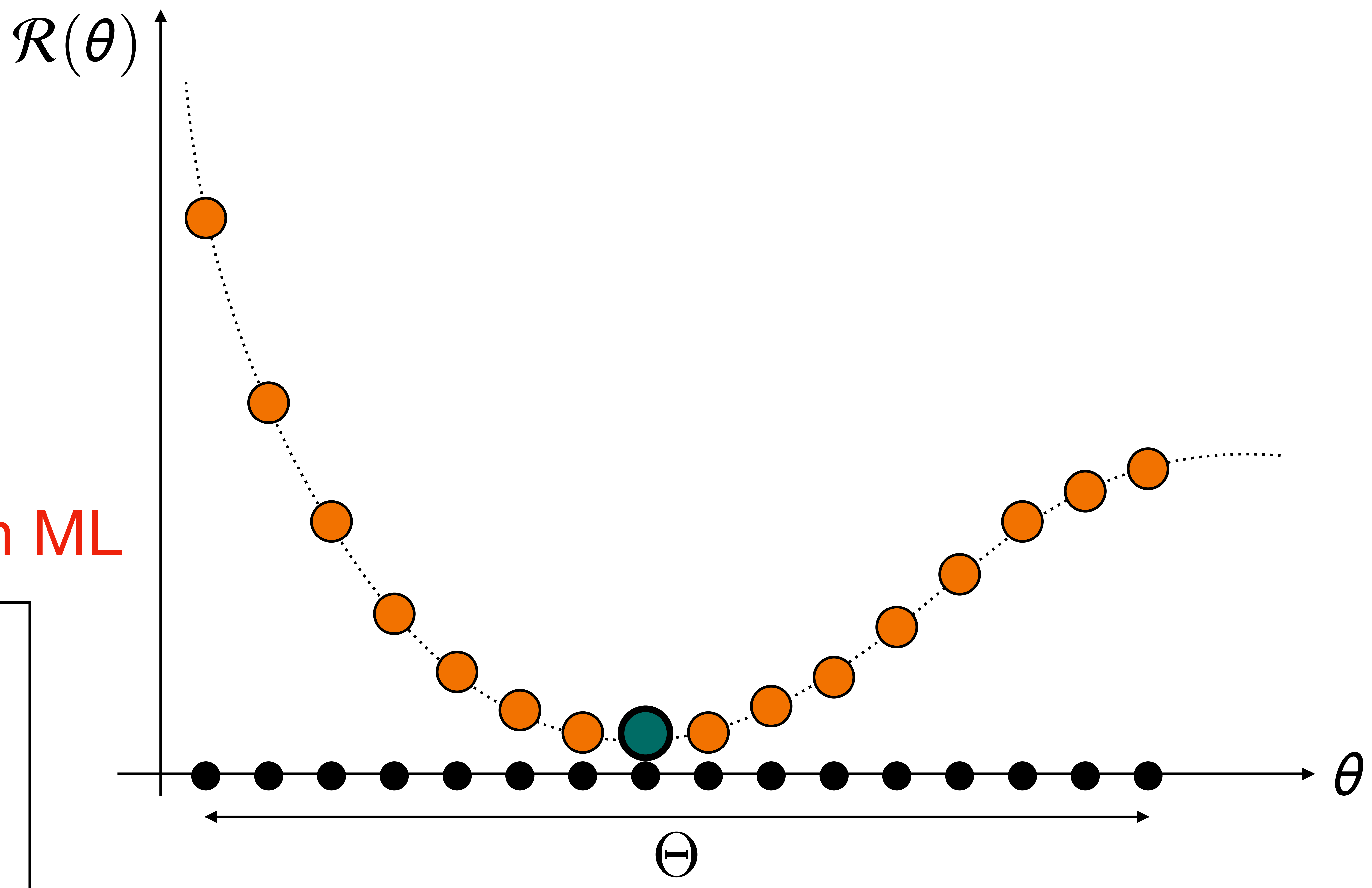
1. Choose a criterion $\mathcal{R}$
2.
3.
4.

Grid search is the standard in ML

Dimensionality issues of sampling Θ



2 parameters   3 parameters



Can be mitigated using Random Search [Bergstra-Bengio '12]
Bayesian methods [Brochu et al. '10]

First order methods for parameter selection

Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}}\, \mathcal{R}(\theta)$

(or close to it)

$$\mathcal{R}(\theta) = \mathcal{C}(\hat{w}_\theta(y)) = (\mathcal{C} \circ \hat{w}_\bullet(y))\,(\theta)$$

$$\mathcal{C} : \mathbb{R}^p \to \mathbb{R}$$

$$\hat{w}_\bullet(y) : \Theta \subseteq \mathbb{R}^l \to \mathbb{R}^p$$

Chain rule

Assuming $\mathcal{C}$ and $\hat{w}_\bullet(y)$ to be differentiable

$$\nabla\mathcal{R}(\theta) = \left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp \nabla\mathcal{C}(\hat{w}_\theta(y))$$

and

$$\nabla\mathcal{R}(\theta^\star) = 0$$

Potential issues

differentiability
access to the cost
size of the Jacobian
approximation stability
convergence (non-convex)

“Hyper”-gradient descent

$$\theta^{k+1} = \theta^k - \rho\nabla\mathcal{R}(\theta^k)$$

possibly **projected** gradient descent on the parameter space

First order methods for parameter selection

Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}}\, \mathcal{R}(\theta)$

(or close to it)

$$\mathcal{R}(\theta) = \mathcal{C}(\hat{w}_\theta(y)) = (\mathcal{C} \circ \hat{w}_{\bullet}(y))(\theta)$$

$$\mathcal{C} : \mathbb{R}^p \to \mathbb{R}$$

$$\hat{w}_{\bullet}(y) : \Theta \subseteq \mathbb{R}^l \to \mathbb{R}^p$$

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and

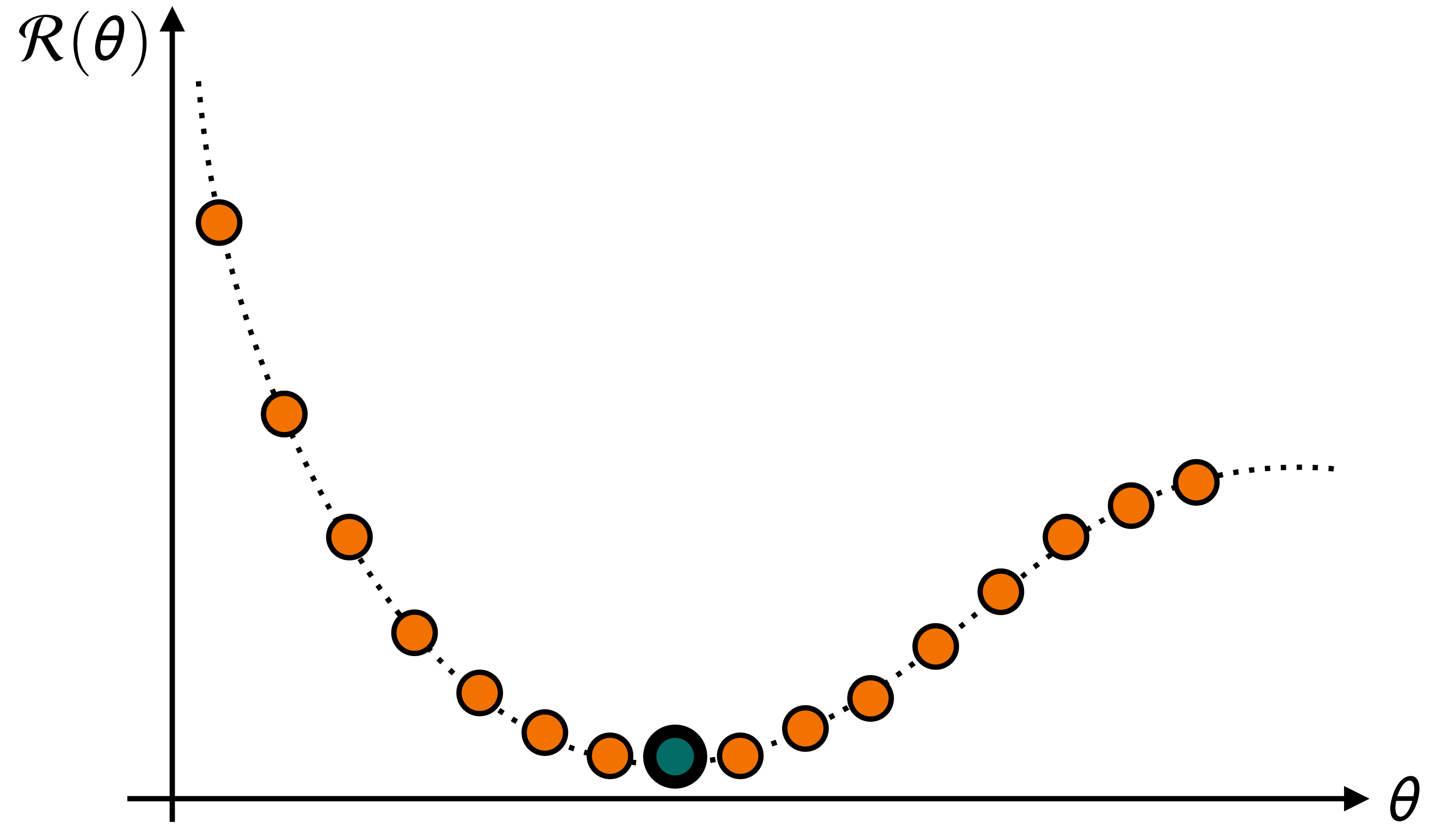
$$\nabla \mathcal{R}(\theta^\star) = 0$$

"Hyper"-gradient descent

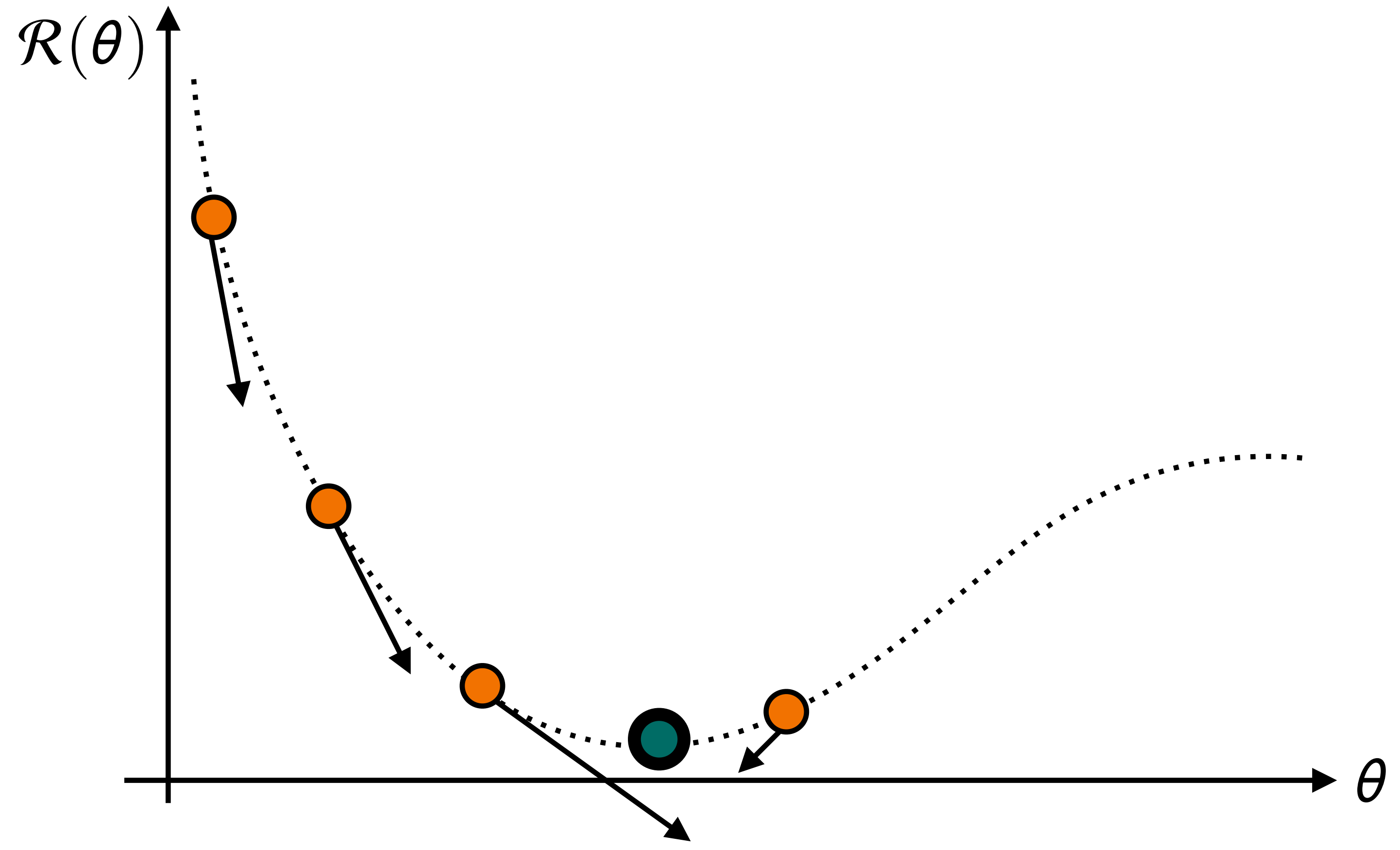
$$\theta^{k+1} = \theta^k - \rho \nabla \mathcal{R}(\theta^k)$$

possibly **projected** gradient descent on the parameter space

Grid search (a.k.a 0-order)



Gradient descent



Implicit differentiation

Q. Bertrand, Q. Klopfenstein, M. Blondel, SV, A. Gramfort, J. Salmon. Implicit differentiation of Lasso-type models for hyperparameter optimization. *ICML*. 2020.
Q. Bertrand, Q. Klopfenstein, M. Blondel, SV, A. Gramfort, J. Salmon. Implicit differentiation for fast hyperparameter selection in non-smooth convex learning. *JMLR*. 2022.

Bilevel problem: implicit differentiation

Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}} \mathcal{R}(\theta)$

(or close to it)

$$\mathcal{R}(\theta) = \mathcal{C}(\hat{w}_\theta(y))$$

- $\mathcal{C}$, $\nabla \mathcal{C}$ easy to compute
- $\hat{w}_\theta$ variational estimator
- $\mathcal{F}$ convex smooth

Bilevel optimization

outer problem

$$\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}} \mathcal{C}(\hat{w}_\theta(y))$$

subject to $\quad \hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\operatorname{argmin}} \mathcal{F}(w, \theta)$

inner problem

$$\nabla \mathcal{R}(\theta) = \left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp \nabla \mathcal{C}(\hat{w}_\theta(y))$$

[Larsen et al. '96] **Fixed point equation** $\quad \nabla_w \mathcal{F}(\hat{w}_\theta(y), \theta) = 0$

$\dfrac{\partial}{\partial \theta}$

$$\nabla^2_{w,\theta} \mathcal{F}(\hat{w}_\theta(y), \theta) + \left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp \nabla^2_w \mathcal{F}(\hat{w}_\theta(y), \theta) = 0$$

assuming invertibility

$$\left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp = -\nabla^2_{w,\theta} \mathcal{F}(\hat{w}_\theta(y), \theta) \left(\nabla^2_w \mathcal{F}(\hat{w}_\theta(y), \theta)\right)^{-1}$$

Smooth case

Kernel-based
[Chapelle et al. '02]
Weighted ridge
[Foo et al. '08]
Image restoration
[Kunish-Pock '13]
Noisy stability
[Pedregosa '16]

Non-smooth

Elastic-net
[Mairal et al. '12]
Lasso
[Dossal et al. '13,
Zou et al. '07]
Generalized Lasso
[V. et al. '13
Tibshirani-Taylor '11]
Partly smooth
[V. et al. '17]
Constrained quad
[Amos-Kolter '17]
Simplex constrained
[Niculae-Blondel '17]

Fast performance for Lasso-like methods

Machine learning

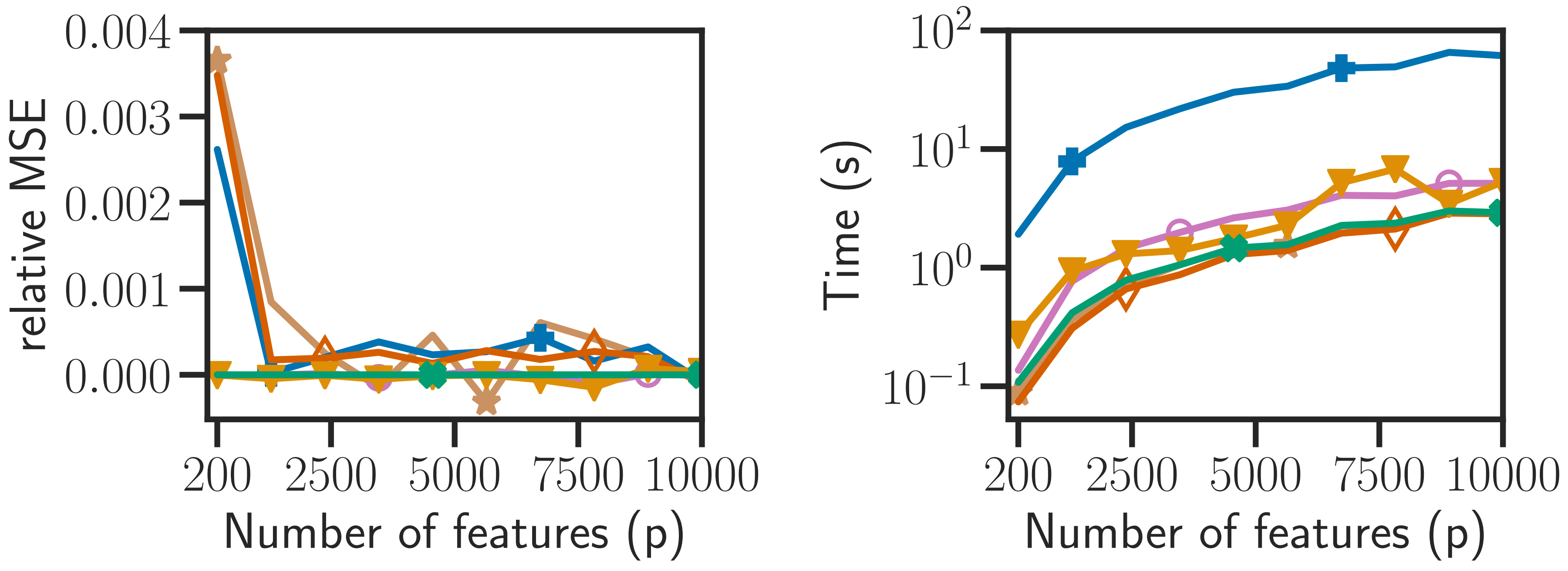
validation set: $y^{\text{val}}, X^{\text{val}}$

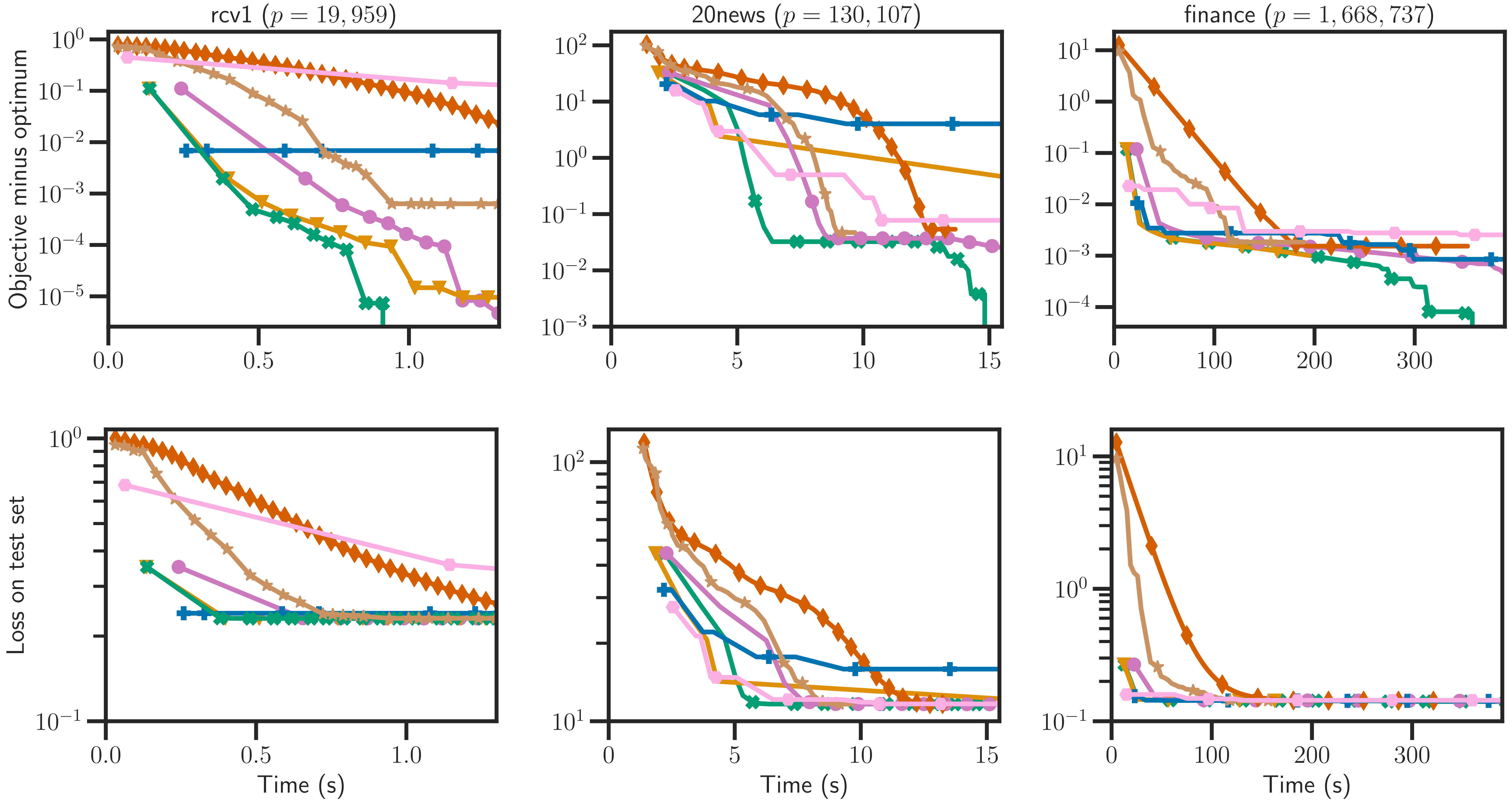
hold-out loss

[Stone-Ramer '65]

$$\mathcal{R}(\theta) = \|y^{\text{val}} - X^{\text{val}} \hat{w}_\theta(y)\|_2^2$$

$\hat{w}_\theta(y)$: Lasso





Computation time

Estimation performance

Estimating a Jacobian

Estimator

$\hat{w}_\theta : \mathbb{R}^n \longrightarrow \mathbb{R}^p$

differentiable

Jacobian

$\text{Jac}_{\hat{w}_\bullet}(y) : \Theta \longrightarrow \mathbb{R}^{p \times l}$

$\text{Jac}_{\hat{w}_\theta} : \mathbb{R}^n \longrightarrow \mathbb{R}^{p \times n}$

$$\text{Jac}_{\hat{w}_\theta}(y) = \begin{pmatrix} \frac{\partial(\hat{w}_\theta)_1}{\partial y_1}(y) & \cdots & \frac{\partial(\hat{w}_\theta)_1}{\partial y_n}(y) \\ \vdots & & \vdots \\ \frac{\partial(\hat{w}_\theta)_p}{\partial y_1}(y) & \cdots & \frac{\partial(\hat{w}_\theta)_p}{\partial y_n}(y) \end{pmatrix} \in \mathbb{R}^{p \times n}$$

Numerical approximation

$$\text{Jac}_{\hat{w}_\theta}(y) \approx \left(\frac{\hat{w}_\theta(y+\delta \mathbf{e}_1) - \hat{w}_\theta(y)}{\delta} \quad \cdots \quad \frac{\hat{w}_\theta(y+\delta \mathbf{e}_n) - \hat{w}_\theta(y)}{\delta} \right)$$

needs $O(nT)$ operations

parameter dimension — cost of evaluating $\hat{w}_\theta(\cdot)$

Symbolic differentiation

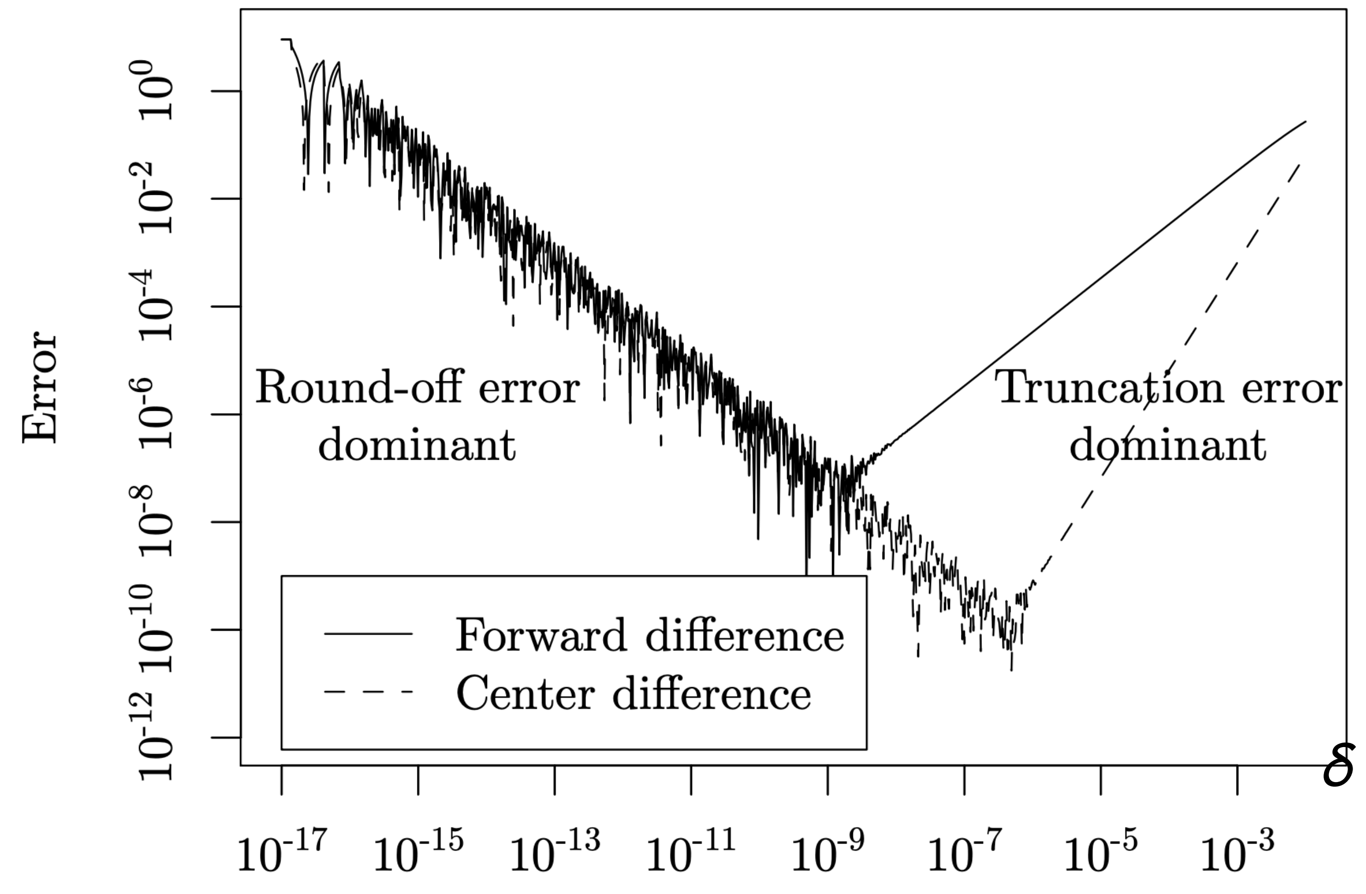
Used by Mathematica, Maple, SymPy, Maxima, Lisp

Ineffective for “complex” programs

$\longrightarrow$ expression swell

Numerical errors

from [Baydin ’18]



$f(x) = 64x(1-x)(1-2x)^2(1-8x+8x^2)^2$

Unstable for low **and** high precision

The SURE way

SV, C. Deledalle, G. Peyré, J. Fadili, C. Dossal. The Degrees of Freedom of Partly Smooth Regularizers. Ann Inst Stat Math. 69(4):791—832. 2017
SV, C. Deledalle, G. Peyré, C. Dossal, J. Fadili. Local Behavior of Sparse Analysis Regularization: Applications to Risk Estimation. Appl Comput Harmon Anal. 35(3):433—451. 2013.

Estimation and prediction risk

Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}}\, \mathcal{R}(\theta)$

(or close to it)

Inverse problems

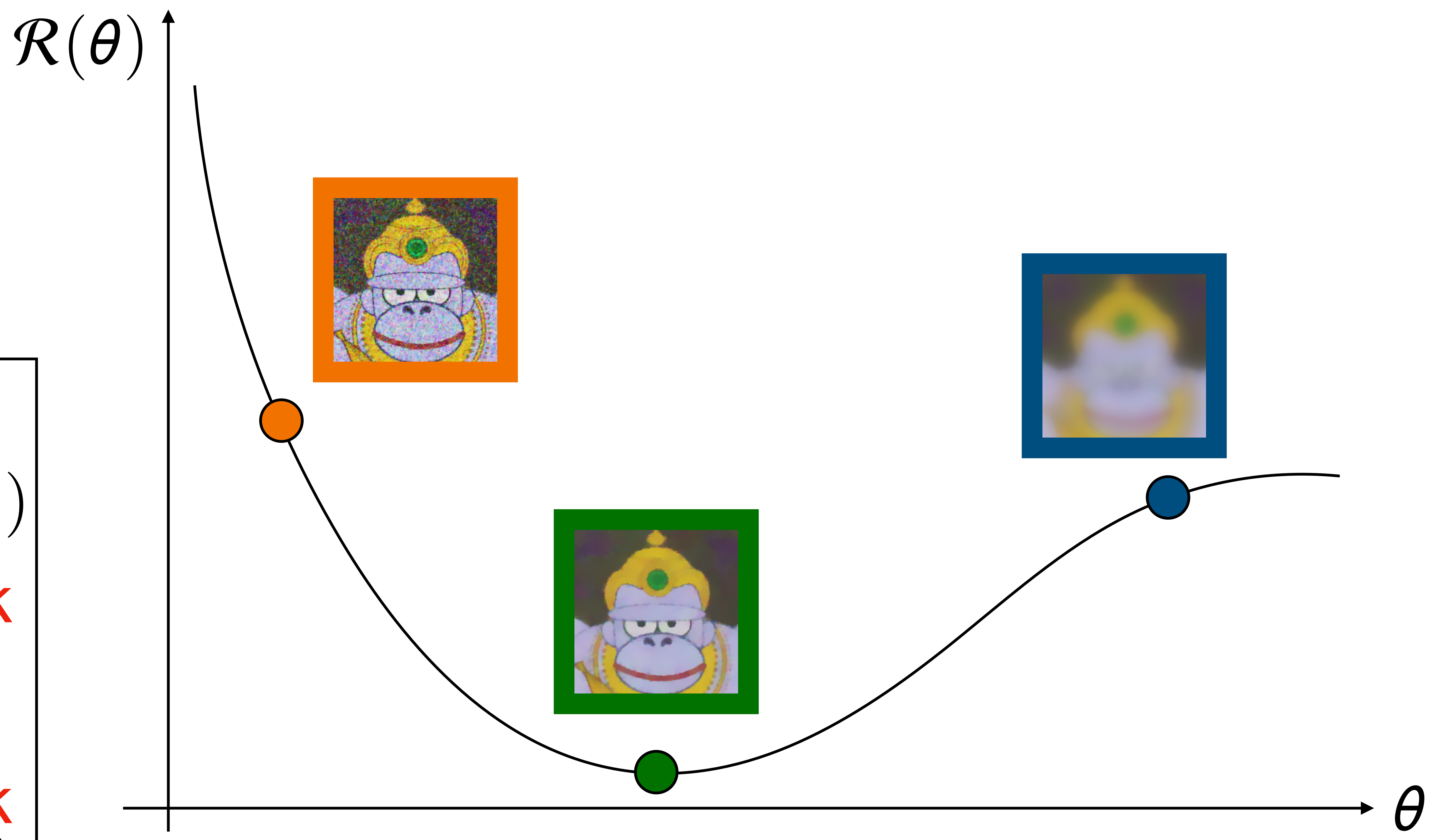
$y = X w_{\text{true}} + \varepsilon \qquad \varepsilon \sim \mathcal{N}(0, \sigma^2 \text{Id})$

estimation risk

$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\| \hat{w}_\theta(y) - w_{\text{true}} \|_2^2 \right)$

prediction risk

$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\| X \hat{w}_\theta(y) - X w_{\text{true}} \|_2^2 \right)$



only **one** observation $y \implies \mathbb{E}_\varepsilon$ is not computable

only one **observation** $y \implies w_{\text{true}}$ is not known

Stein Unbiased Risk Estimation — SURE

Inverse problems

$$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \text{Id})$$

Prediction

$$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$$

Prediction risk

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\| \hat{\mu}_\theta(y) - X w_{\text{true}} \|_2^2 \right)$$

Degrees of freedom [Efron '86]

$$\text{df}_\theta(y) = \sum_{i=1}^{n} \frac{\text{cov}(\hat{\mu}_\theta(y)_i, y_i)}{\sigma^2}$$

→

Cp [Mallows '73]
AIC [Akaike '73]
BIC [Schwarz '78]
GCV [Craven-Wahba '79]
SURE [Stein '81]

Examples

Ordinary least square

$$\text{df}_\theta(y) = p$$

Lasso [Dossal et al. '13, Zou et al. '07]

$$\text{df}_\theta(y) = \| \hat{w}_\theta(y) \|_0 = |\text{supp}(\hat{w}_\theta(y))|$$

Stein's lemma

[Stein '81]

If $\hat{\mu}_\theta$ weakly differentiable

Empirical degrees of freedom

$$\widehat{\text{df}}_\theta(y) = \text{div}(\hat{\mu}_\theta(y)) = \sum_{i=1}^{n} \frac{\partial (\hat{\mu}_\theta)_i}{\partial y_i}(y)$$

$$\mathbb{E}_\varepsilon(\widehat{\text{df}}_\theta(y)) = \text{df}_\theta(y)$$

Stein Unbiased Risk Estimation

[Stein '81]

If $\hat{\mu}_\theta$ weakly differentiable

$$\text{SURE}_\theta(y) = \| y - \hat{\mu}_\theta(y) \|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\text{df}}_\theta(y)$$

$$\mathbb{E}_\varepsilon(\text{SURE}_\theta(y)) = \mathcal{R}(\theta)$$

🥴 requires the noise variance

SURE for smooth regularized least square

Inverse problems

$$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \mathrm{Id})$$

Prediction

$$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$$

Prediction risk

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\|\hat{\mu}_\theta(y) - X w_{\text{true}}\|_2^2 \right)$$

Degrees of freedom and SURE

$$\widehat{\mathrm{df}}_\theta(y) = \mathrm{div}(\hat{\mu}_\theta(y)) = \sum_{i=1}^{n} \frac{\partial (\hat{\mu}_\theta)_i}{\partial y_i}(y)$$

$$\mathrm{SURE}_\theta(y) = \|y - \hat{\mu}_\theta(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta(y)$$

$$\mathbb{E}_\varepsilon(\mathrm{SURE}_\theta(y)) = \mathcal{R}(\theta)$$

Smooth regularised least-square

$$\hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\mathrm{argmin}} \frac{1}{2}\|y - X w\|_2^2 + \theta J(w)$$

First order conditions

$$X^\top (X \hat{w}_\theta(y) - y) + \theta \nabla J(\hat{w}_\theta(y)) = 0$$

Implicit function theorem

$$\Gamma_\theta(y) = X^\top X + \theta \nabla^2 J(\hat{w}_\theta(y)) \longrightarrow \mathrm{Jac}_{\hat{\mu}_\theta}(y) = X \Gamma_\theta(y)^{-1} X^\top$$

SURE for regularized least square

Inverse problems

$$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \text{Id})$$

Prediction

$$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$$

Prediction risk

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\|\hat{\mu}_\theta(y) - X w_{\text{true}}\|_2^2 \right)$$

Degrees of freedom and SURE

$$\widehat{\text{df}}_\theta(y) = \text{div}(\hat{\mu}_\theta(y)) = \sum_{i=1}^{n} \frac{\partial (\hat{\mu}_\theta)_i}{\partial y_i}(y)$$

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~~Smooth~~ regularised least-square

$$\hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\text{argmin}} \frac{1}{2}\|y - Xw\|_2^2 + \theta J(w)$$

Theorem [V. et al. '13,17]

When J is regular enough, $\text{Jac}_{\hat{\mu}_\theta(y)}(y)$ is computable *a.e.* in closed form

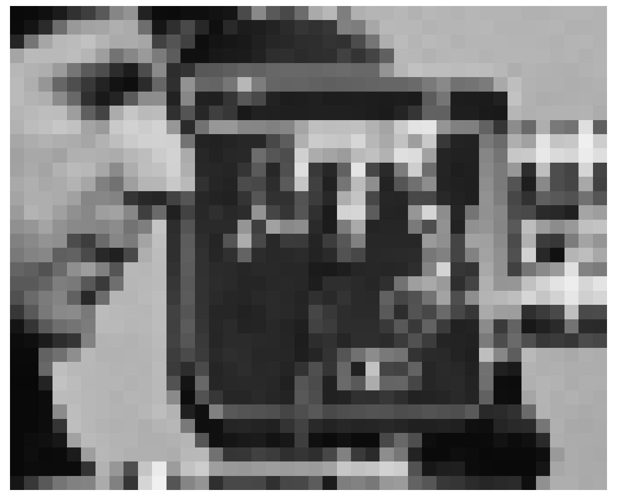
Generalizes [Yuan-Lin '06, Dossal et al. '12, Tibshirani-Taylor '12, ...]

Example: SURE Grid search

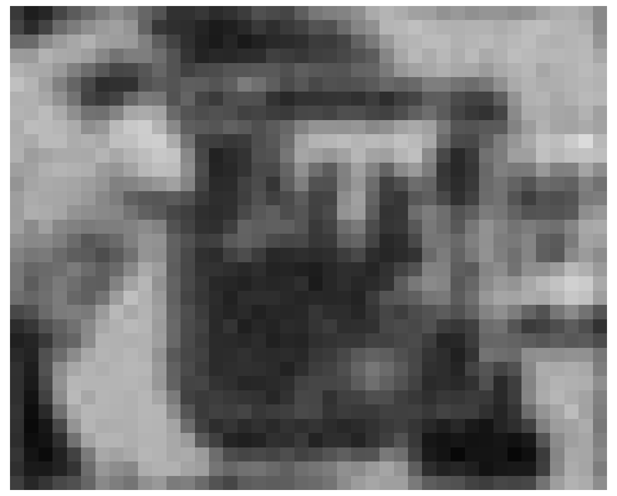
Anisotropic Total Variation

$$J(w) = \|\nabla_{2D} w\|_1$$

X Gaussian convolution

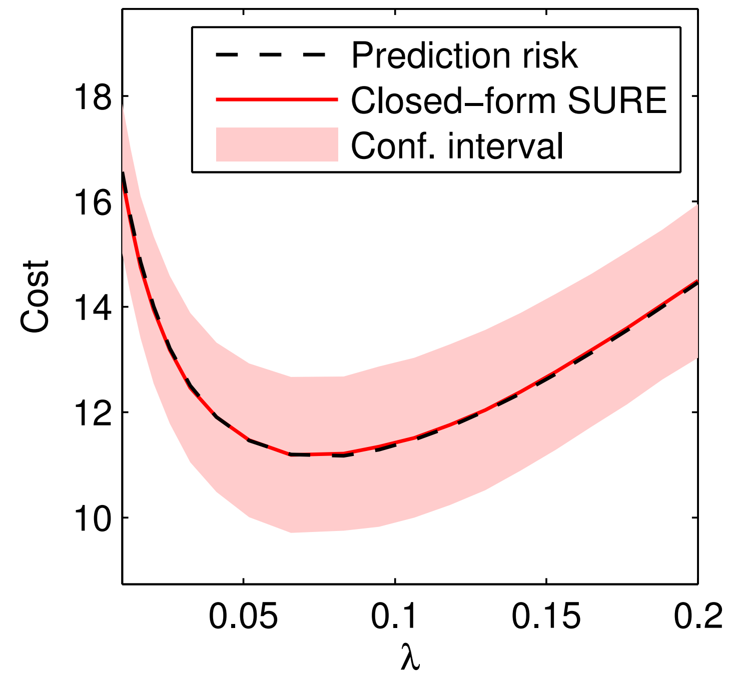


original



blurred

optimal



Explicit SURE: shortcomings

Inverse problems

$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \text{Id})$

Prediction

$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$

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Degrees of freedom and SURE

$$\widehat{\text{df}}_\theta(y) = \text{div}(\hat{\mu}_\theta(y)) = \sum_{i=1}^{n} \frac{\partial (\hat{\mu}_\theta)_i}{\partial y_i}(y)$$

$$\text{SURE}_\theta(y) = \| y - \hat{\mu}_\theta(y) \|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\text{df}}_\theta(y)$$

$$\mathbb{E}_\varepsilon(\text{SURE}_\theta(y)) = \mathcal{R}(\theta)$$

Pb 1: expectation VS realization

only **one** observation $y \implies \mathbb{E}_\varepsilon$ is not computable

(Mostly stable because expectation of a low dimensional quantity with a high dimensional variable)

Pb 2: computational tractability

$\widehat{\text{df}}_\theta(y) = \text{trace}(\text{Jac}_{\hat{\mu}_\theta}(y))$ potentially large

$\longrightarrow$ Monte Carlo SURE

Pb 3: convergence

$w_\theta^{(k)}(y) \xrightarrow{?} \hat{w}_\theta(y)$

stability

$\text{Jac}_{w_\theta^{(k)}}(y) \xrightarrow{?} \text{Jac}_{\hat{w}_\theta}(y)$

very high precision required

Automatic differentiation

J. Bolte, E. Pauwels, SV. Automatic differentiation of non-smooth iterative solvers. 2022

Explicit SURE: shortcomings

Inverse problems

$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \text{Id})$

Prediction

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Degrees of freedom and SURE

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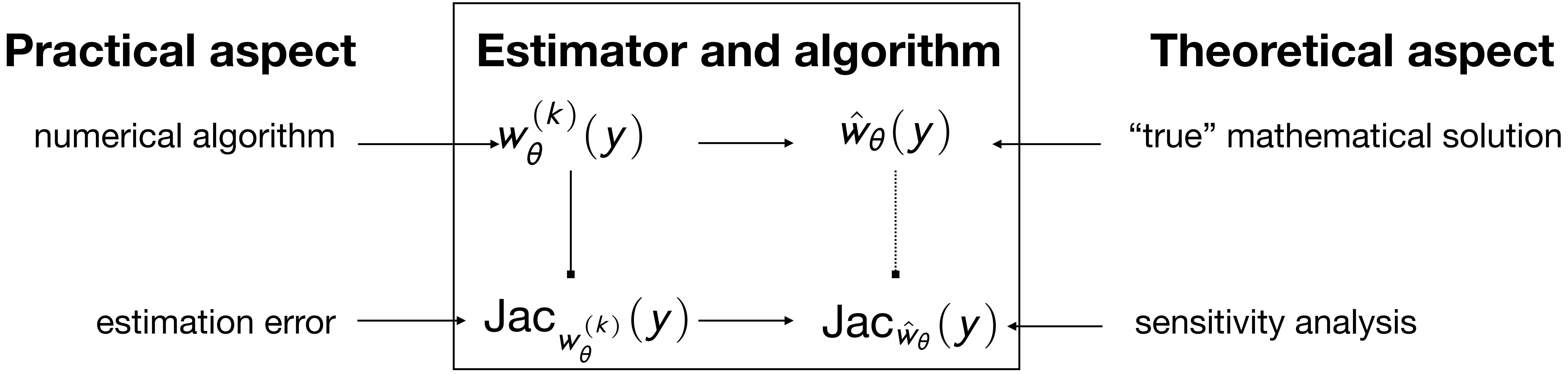
$$\mathbb{E}_\varepsilon(\text{SURE}_\theta(y)) = \mathcal{R}(\theta)$$



Convergence of functions does not imply convergence of derivatives!

Automatic differentiation: forward mode

Function

$$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$$\mathrm{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$$

$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

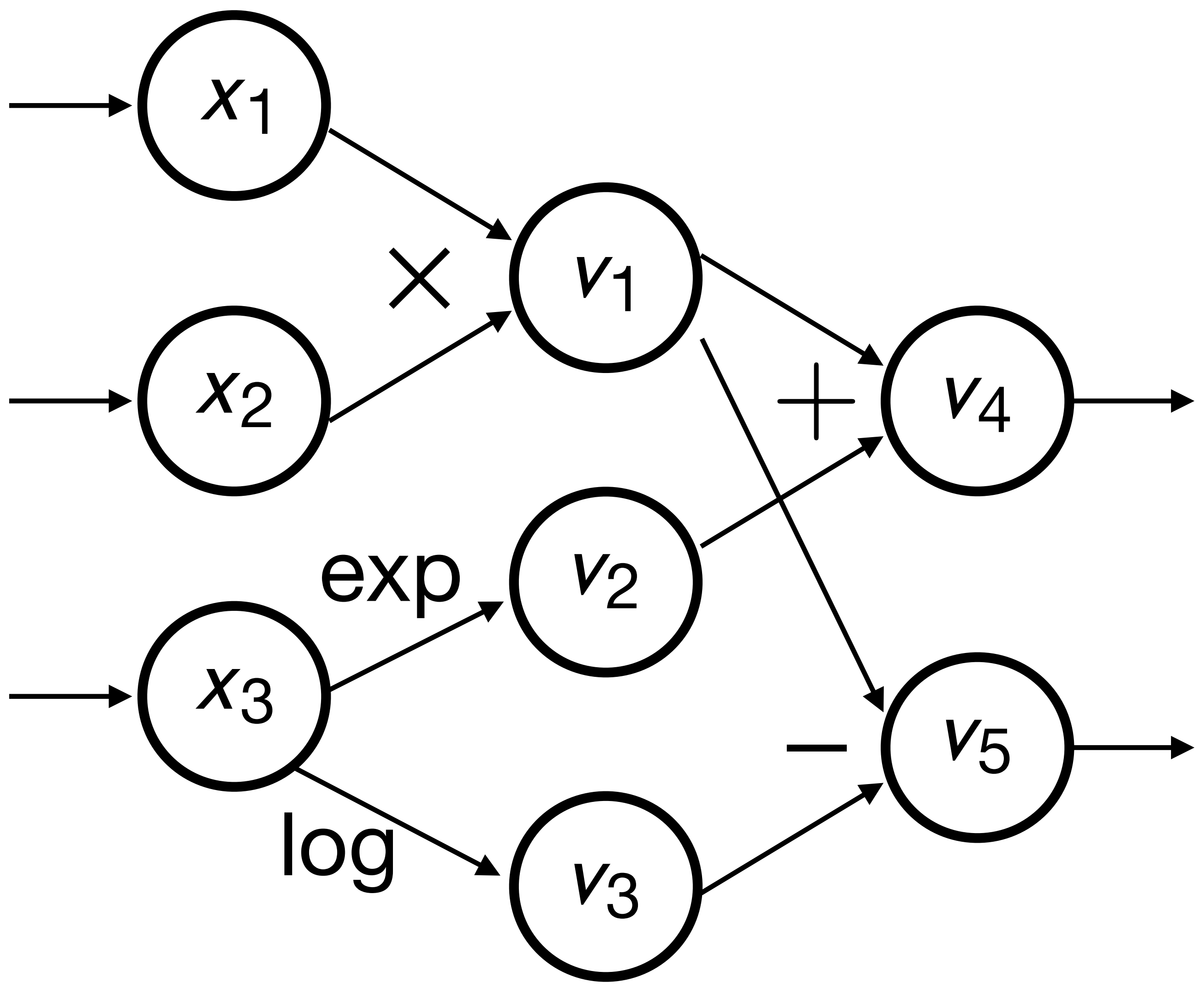
$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

Computer program

```
def f(x1, x2, x3):
    v1 = x1 * x2
    v2 = exp(x3)
    v3 = log(x3)
    v4 = v1 + v2
    v5 = v1 - v3
    return (v4, v5)
```

Forward Tangent Program

Computational graph [Bauer '74]



Inspired by [Baydin '18]

Automatic differentiation: forward mode

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Jacobian

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$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

Computer program

1.00 2.00 3.00

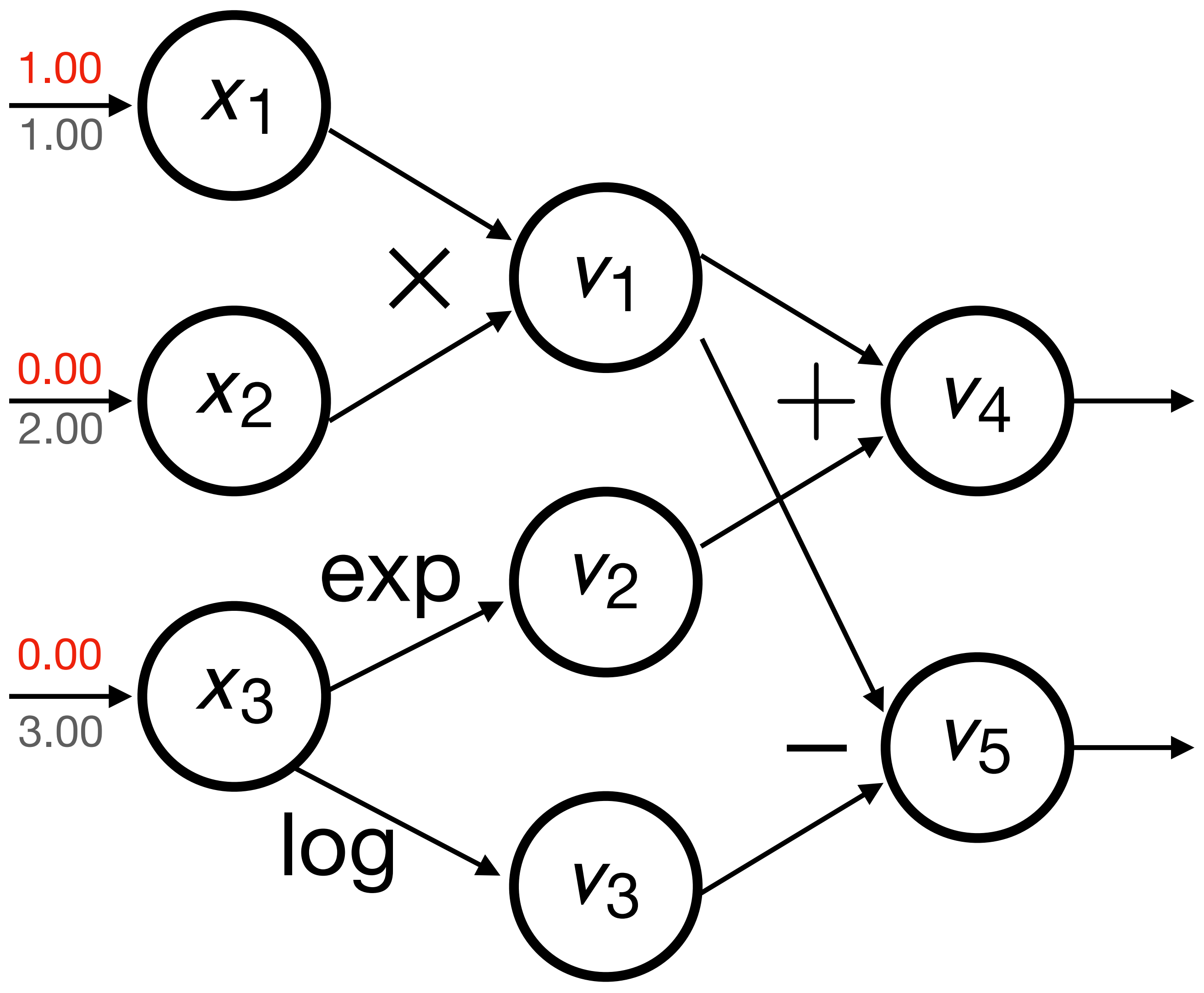
```
def f(x1, x2, x3):
```

Forward Tangent Program

1.00 0.00 0.00

```
def df(dx1, dx2, dx3):
```

Computational graph [Bauer '74]



Inspired by [Baydin '18]

Automatic differentiation: forward mode

Function

$$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$$\text{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$$

$$\text{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

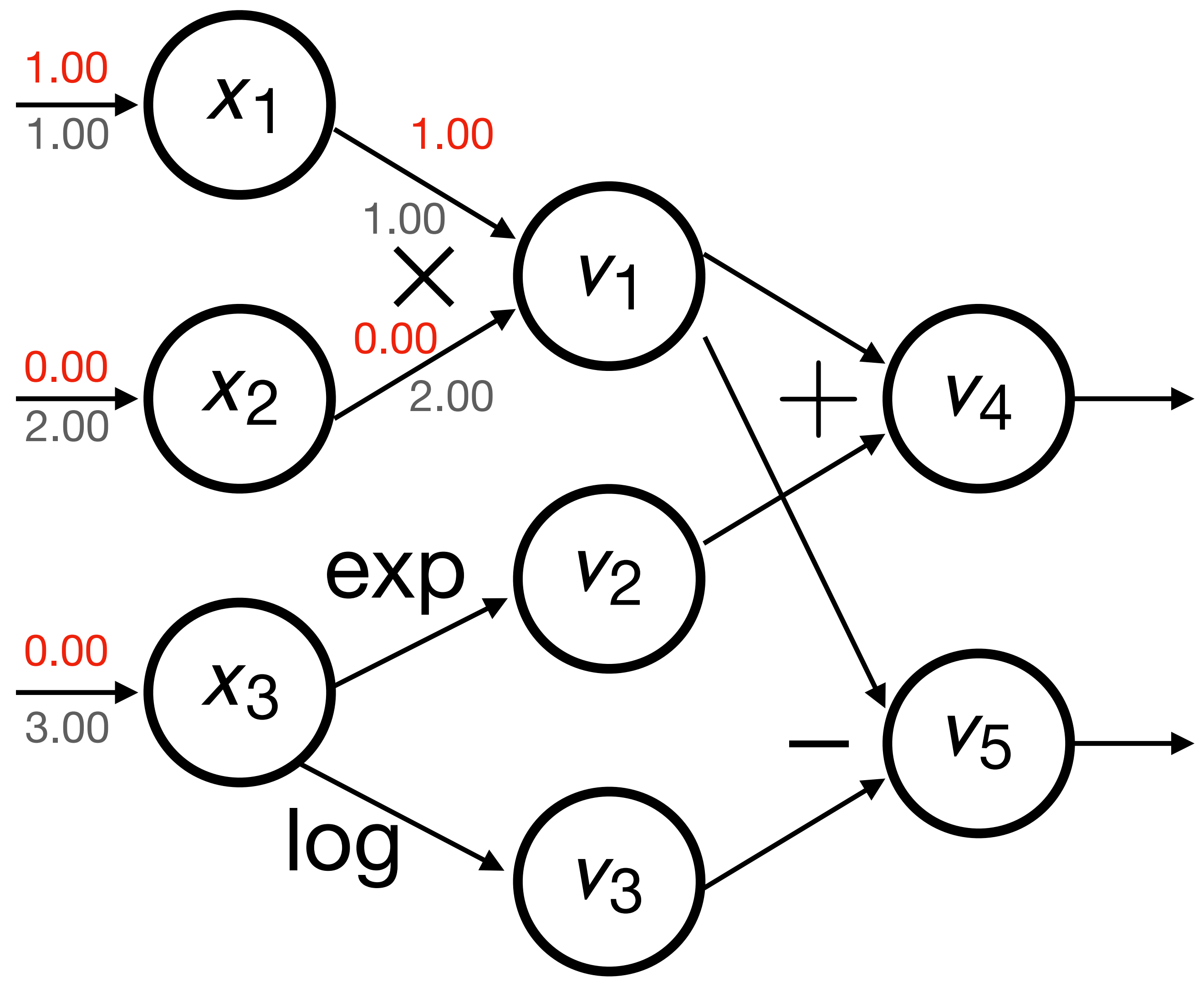
Computer program

```
      1.00  2.00  3.00
def f(x1,   x2,   x3):
    v1 = x1 * x2            2.00
```

Forward Tangent Program

```
       1.00  0.00  0.00
def df(dx1,  dx2,  dx3):
    dv1 = dx1 * x2 + dx1 * x2    2.00
```

Computational graph [Bauer '74]



Inspired by [Baydin '18]

Automatic differentiation: forward mode

Function

$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$\mathrm{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$

$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

Computer program

1.00 2.00 3.00

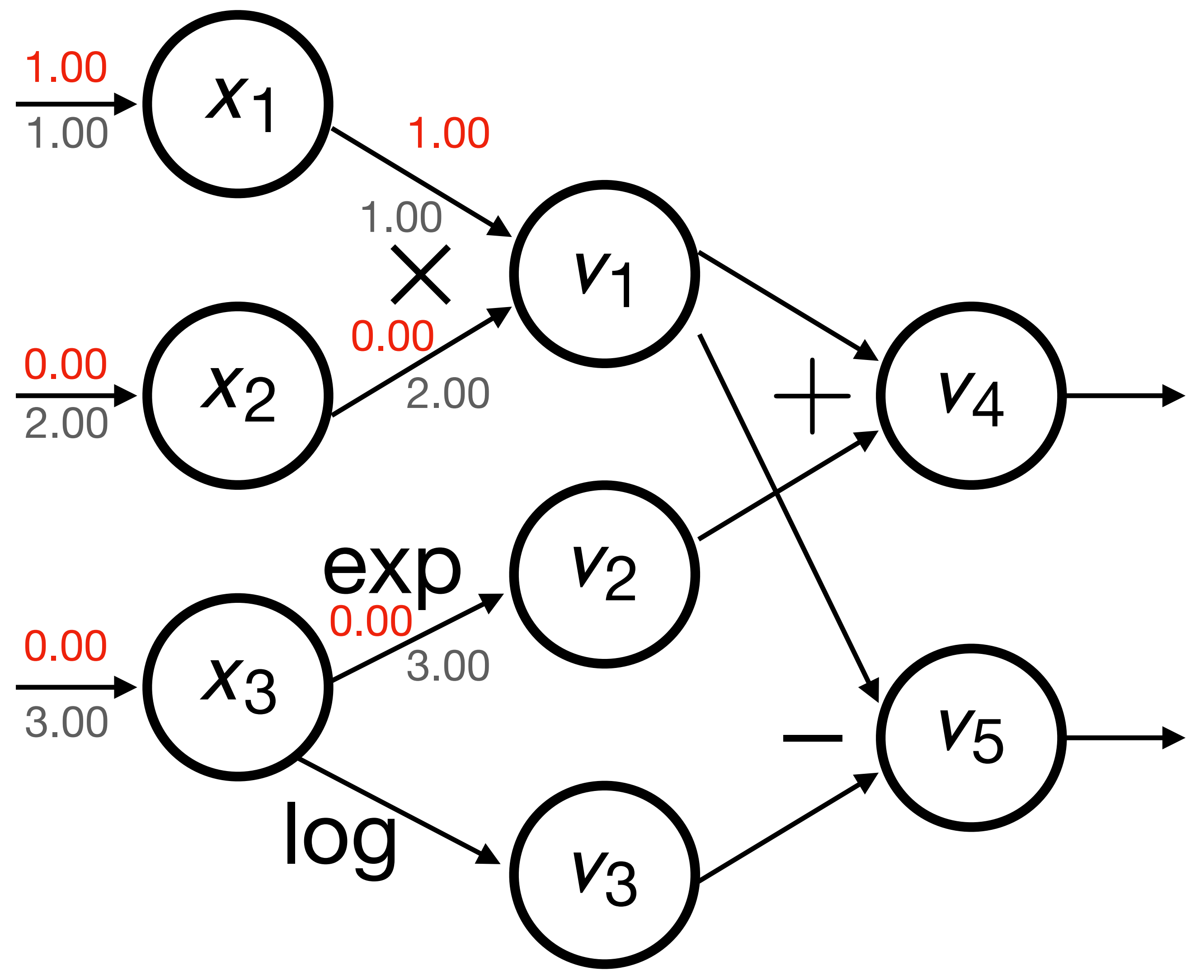
```
def f(x1, x2, x3):
    v1 = x1 * x2          2.00
    v2 = exp(x3)          20.08
```

Forward Tangent Program

1.00 0.00 0.00

```
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
```

Computational graph [Bauer '74]



Inspired by [Baydin '18]

Automatic differentiation: forward mode

Function

$$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$$\mathrm{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$$

$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

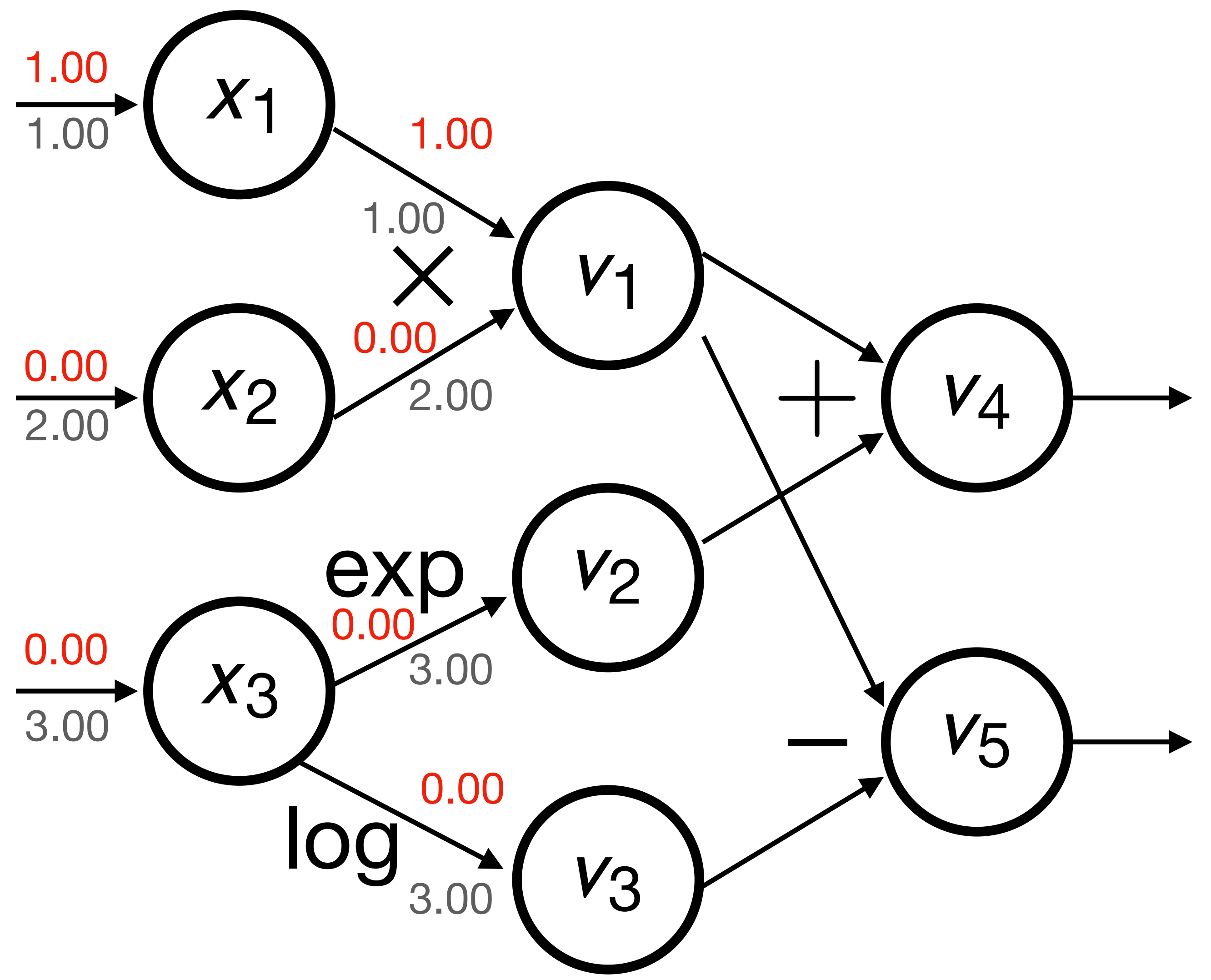
Computer program

```
         1.00  2.00  3.00
def f(x1, x2, x3):
    v1 = x1 * x2          2.00
    v2 = exp(x3)          20.08
    v3 = log(x3)          0.48
```

Forward Tangent Program

```
          1.00  0.00  0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
    dv3 = dx3 / x3                0.00
```

Computational graph [Bauer '74]



Automatic differentiation: forward mode

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$$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$$\mathrm{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$$

$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

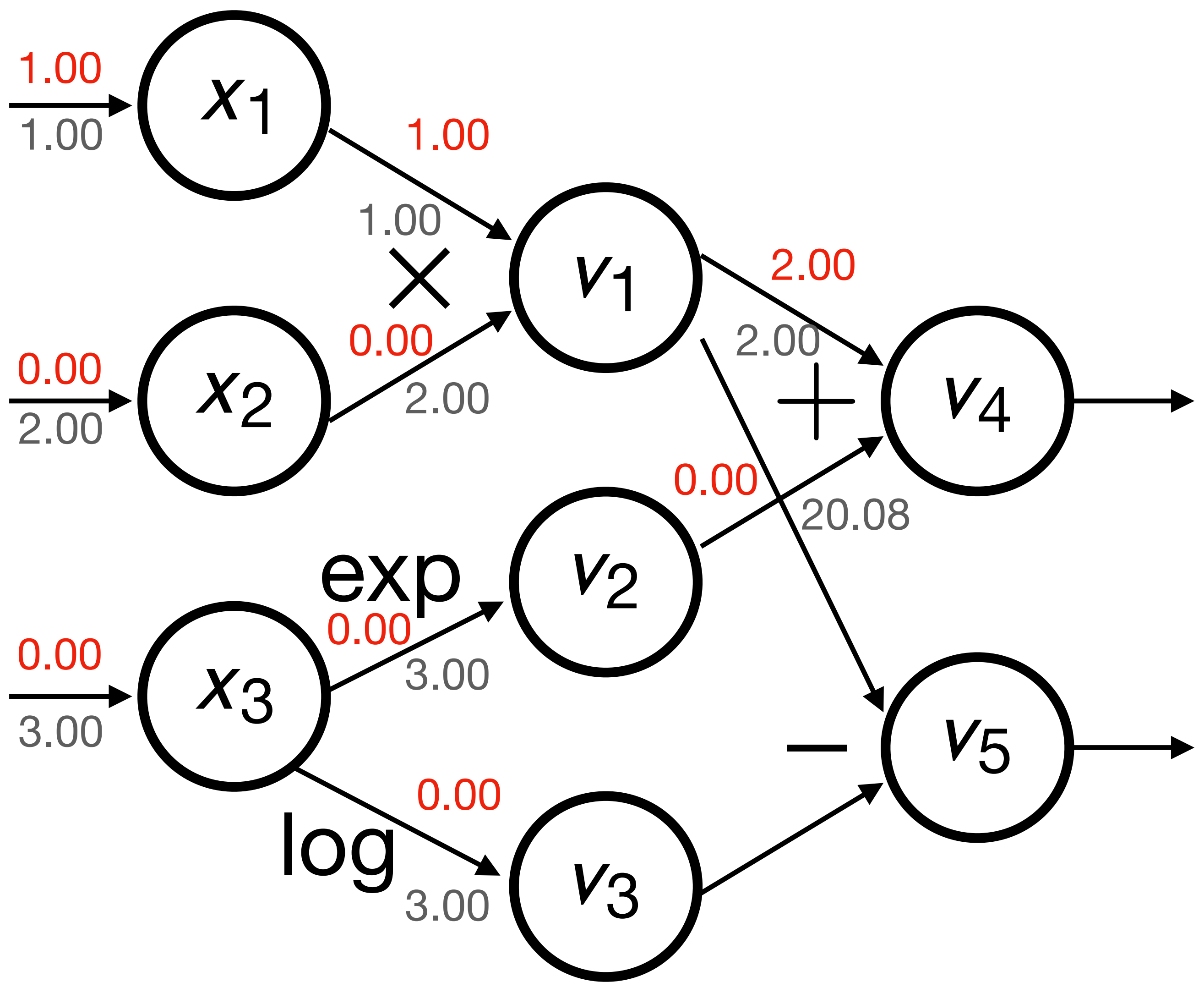
Computer program

```
        1.00  2.00  3.00
def f(x1, x2, x3):
    v1 = x1 * x2          2.00
    v2 = exp(x3)          20.08
    v3 = log(x3)          0.48
    v4 = v1 + v2          22.08
```

Forward Tangent Program

```
         1.00  0.00  0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
    dv3 = dx3 / x3                0.00
    dv4 = dv1 + dv2               2.00
```

Computational graph [Bauer '74]



Inspired by [Baydin '18]

Automatic differentiation: forward mode

Function

$$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

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$$\text{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

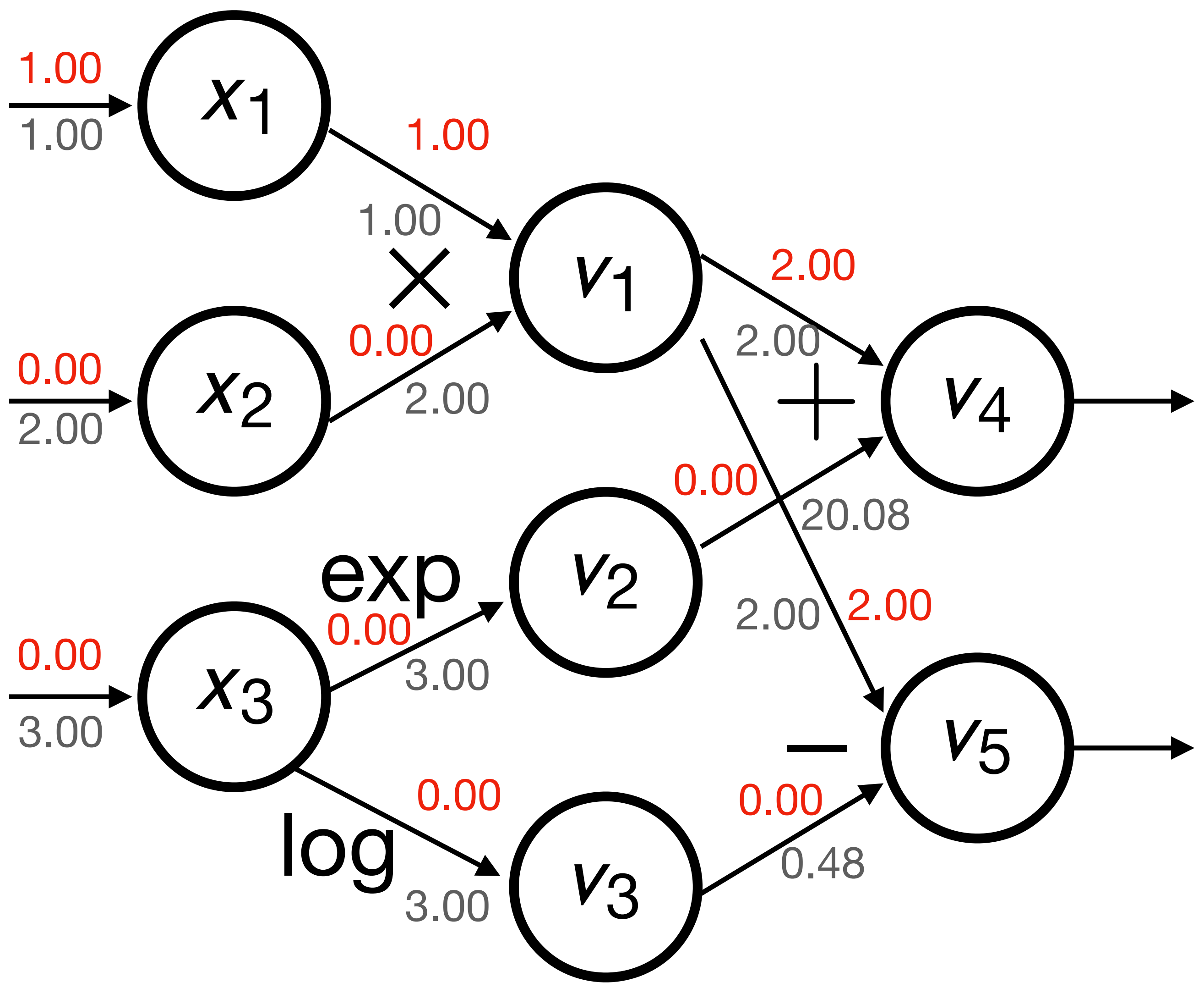
Computer program

```
      1.00  2.00  3.00
def f(x1, x2, x3):
    v1 = x1 * x2        2.00
    v2 = exp(x3)        20.08
    v3 = log(x3)        0.48
    v4 = v1 + v2        22.08
    v5 = v1 - v3        2.08
```

Forward Tangent Program

```
       1.00  0.00  0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
    dv3 = dx3 / x3                0.00
    dv4 = dv1 + dv2               2.00
    dv5 = dv1 - dv3               2.00
```

Computational graph [Bauer '74]



Automatic differentiation: forward mode

Function

$$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$$\mathrm{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$$

$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

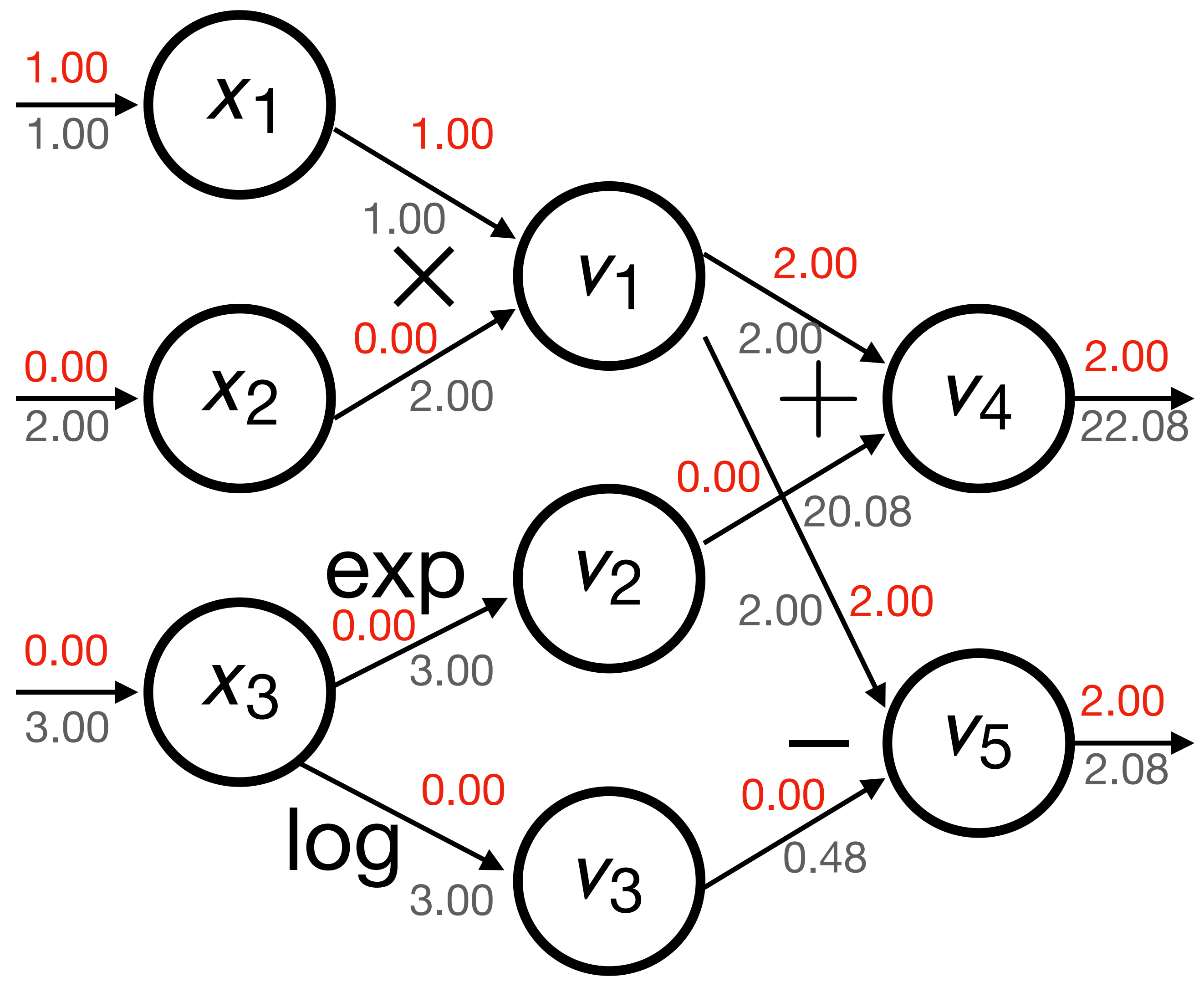
Computer program

```
        1.00   2.00   3.00
def f(x1, x2, x3):
    v1 = x1 * x2              2.00
    v2 = exp(x3)              20.08
    v3 = log(x3)              0.48
    v4 = v1 + v2              22.08
    v5 = v1 - v3              2.08
    return (v4, v5)  (22.08, 2.08)
```

Forward Tangent Program

```
         1.00   0.00   0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
    dv3 = dx3 / x3                0.00
    dv4 = dv1 + dv2               2.00
    dv5 = dv1 - dv3               2.00
    return (dv4, dv5)      (2.00, 2.00)
```

Computational graph [Bauer '74]



Automatic differentiation: forward mode

Function

$$f : \mathbb{R}^p \rightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$$\text{Jac}_f : \mathbb{R}^p \rightarrow \mathbb{R}^{n \times p}$$

$$\text{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

- Computing the full Jacobian requires p calls to tangent program
- No memory requirement
- Performant when $p < n$

[Wengert '64, Griewank '89]

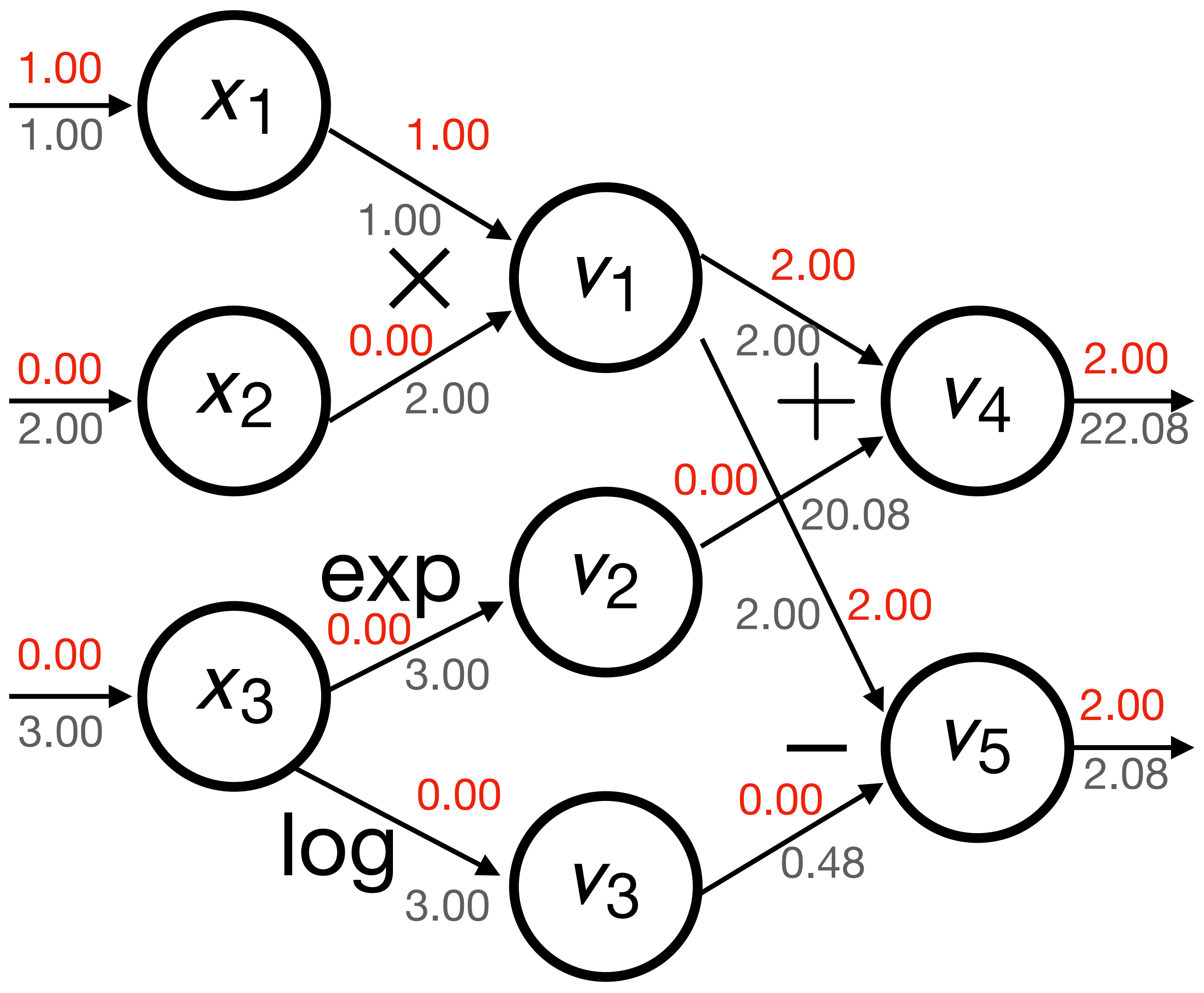
Computer program

```
       1.00  2.00  3.00
def f(x1, x2, x3):
    v1 = x1 * x2            2.00
    v2 = exp(x3)            20.08
    v3 = log(x3)            0.48
    v4 = v1 + v2            22.08
    v5 = v1 - v3            2.08
    return (v4, v5)         (22.08, 2.08)
```

Forward Tangent Program

```
        1.00  0.00  0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
    dv3 = dx3 / x3                0.00
    dv4 = dv1 + dv2               2.00
    dv5 = dv1 - dv3               2.00
    return (dv4, dv5)             (2.00, 2.00)
```

Computational graph [Bauer '74]



Forward automatic differentiation

=

Forward derivative accumulation

=

Tangent linear mode

=

Line-to-line derivation

=

Jacobian-vector product

$\text{Jac}_f(x) \cdot z$

$\neq$

~~Backpropagation~~

Note that in practice the forward tangent program need to be implemented in the same function (variables accessibility)

Inspired by [Baydin '18]

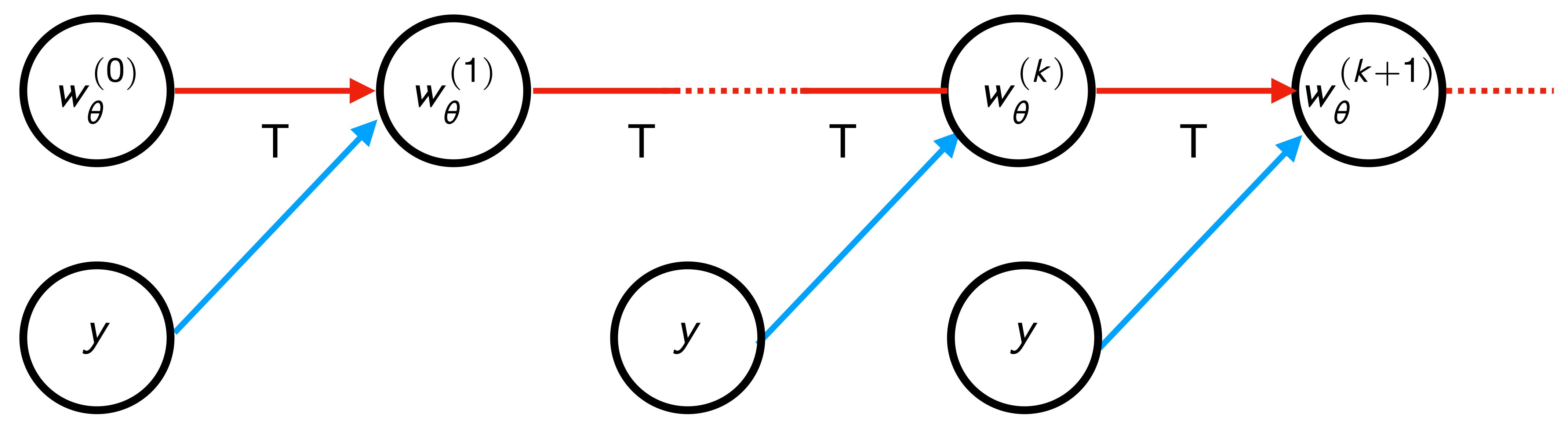
Estimating a Jacobian of iterative estimator

Iterative estimators $w_\theta^{(k)}(y)$

$$\mathrm{T} : \mathbb{R}^p \times \mathbb{R}^n \to \mathbb{R}^p$$

$$\begin{cases} w_\theta^{(k)}(y) \xrightarrow{k \to +\infty} \hat{w}_\theta(y) \\ w_\theta^{(k+1)}(y) = \mathrm{T}(w_\theta^{(k)}(y), y) \end{cases}$$

Computational graph



Chain rule

$$\mathrm{Jac}_{w_\theta^{k+1}}(y) = \partial_1 \mathrm{T}(w_\theta^k(y), y) \cdot \mathrm{Jac}_{w_\theta^k(y)}(y) + \partial_2 \mathrm{T}(w_\theta^k(y), y)$$

$p \times n$ $\quad$ $p \times p$ $\quad$ $p \times n$ $\quad$ $p \times n$

Forward differentiation "Jacobian-vector product"

$$\begin{cases} w_\theta^{(k+1)}(y) & = \mathrm{T}(w_\theta^{(k)}(y), y) \\ \mathrm{d}w_\theta^{(k+1)}(y) & = \partial_1 \mathrm{T}(w_\theta^k(y), y) \cdot \mathrm{d}w_\theta^{(k+1)}(y) + \partial_2 \mathrm{T}(w_\theta^k(y), y)\delta \end{cases}$$

Well-foundness of iterative differentiation

Iterative estimators $w_\theta^{(k)}(y)$

$$\mathrm{T} : \mathbb{R}^p \times \mathbb{R}^n \to \mathbb{R}^p$$

$$\begin{cases} w_\theta^{(k)}(y) \xrightarrow{k \to +\infty} \hat{w}_\theta(y) \\ w_\theta^{(k+1)}(y) = \mathrm{T}(w_\theta^{(k)}(y), y) \end{cases}$$

Forward differentiation "Jacobian-vector product"

$$w_\theta^{(k+1)}(y) = \mathrm{T}(w_\theta^{(k)}(y), y)$$

$$\mathrm{d}w_\theta^{(k+1)}(y) = \partial_1 \mathrm{T}(w_\theta^k(y), y) \cdot \mathrm{d}w_\theta^{(k+1)}(y) + \partial_2 \mathrm{T}(w_\theta^k(y), y)\delta$$

Theorem [Bolte, Pauwels, V '22]

If T is loc. Lipschitz and its *conservative Jacobian* is a contraction, then for almost all y,

$$\lim_{k \to +\infty} \mathrm{d}w_\theta^{(k)}(y) = \frac{\partial \hat{w}_\theta(y)}{\partial y} \cdot \delta$$

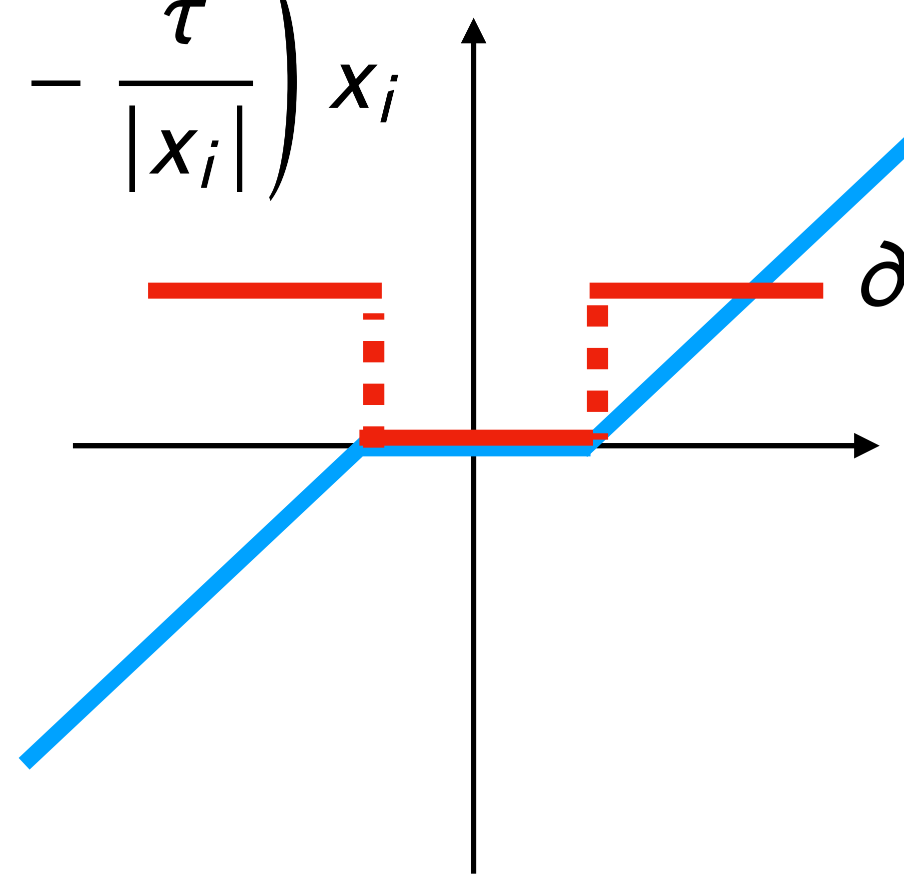
Forward differentiation of a Lasso solver

Lasso

$$\hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\operatorname{argmin}} \frac{1}{2}\|y - Xw\|_2^2 + \theta\|w\|_1$$

Soft-thresholding

$$\operatorname{prox}_{\tau\|\cdot\|_1}(x)_i = \min\left(0, 1 - \frac{\tau}{|x_i|}\right) x_i$$



Iterative soft-thresholding (Forward-Backward)

$$w_\theta^{(k+1)}(y) = \operatorname{prox}_{\tau\theta\|\cdot\|_1}(w_\theta^{(k)}(y) - \tau X^\top(Xw_\theta^{(k)}(y) - y))$$

If $\tau < 2/\|X\|^2$, $w_\theta^{(k)}(y) \to \hat{w}_\theta(y)$

Derivative of Forward-Backward

$$\begin{aligned}
\partial_1 \mathrm{T}(w, y) &= \mathrm{Jac}_{\operatorname{prox}_{\tau\theta\|\cdot\|_1}}(w - \tau X^\top(Xw - y)) \cdot \mathrm{Jac}_{w \mapsto w - \tau X^\top(Xw - y)}(w) \\
&= \partial\operatorname{prox}_{\tau\theta\|\cdot\|_1}(w - \tau X^\top(Xw - y)) \cdot (\mathrm{Id} - \tau X^\top X) \\
\partial_2 \mathrm{T}(w, y) &= \mathrm{Jac}_{\operatorname{prox}_{\tau\theta\|\cdot\|_1}}(w - \tau X^\top(Xw - y)) \cdot \mathrm{Jac}_{y \mapsto w - \tau X^\top(Xw - y)}(y) \\
&= \partial\operatorname{prox}_{\tau\theta\|\cdot\|_1}(w - \tau X^\top(Xw - y)) \cdot \tau X
\end{aligned}$$

The SUGAR way

B. Pascal, SV, N. Pustelnik, P. Abry. Automated data-driven selection of the hyperparameters for Total-Variation based texture segmentation. 2020.
C. Deledalle, SV, J. Fadili, G. Peyré. Stein Unbiased GrAdient estimator of the Risk (SUGAR) for multiple parameter selection. SIAM J Imaging Sci. 7(4):2448—2487. 2014.
C. Deledalle, SV, G. Peyré, J. Fadili, C. Dossal. Proximal Splitting Derivatives for Risk Estimation. *NCMIP*. 2012.

Fifty shades of SURE

Closed-form SURE [Stein '81]

$$\mathrm{SURE}_\theta(y) = \|y - \hat{\mu}_\theta(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta(y) \qquad \widehat{\mathrm{df}}_\theta(y) = \mathrm{trace}(\mathrm{Jac}_{\hat{\mu}_\theta}(y))$$

Issue: dimensionality of the Jacobian

$$\mathbb{E}_z\left(\widehat{\mathrm{df}}_\theta^{\mathrm{MC}}(y)\right) = \widehat{\mathrm{df}}_\theta(y)$$

Monte-Carlo SURE [Ramani et al. '08]

$$z \sim \mathcal{N}(0, \mathrm{Id})$$

$$\mathrm{SURE}_\theta^{\mathrm{MC}}(y) = \|y - \hat{\mu}_\theta(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta^{\mathrm{MC}}(y) \qquad \widehat{\mathrm{df}}_\theta^{\mathrm{MC}}(y) = \langle \mathrm{Jac}_{\hat{\mu}_\theta}(y) z, \, z \rangle$$

Issue: accessibility of the true Jacobian

need proof
of convergence

Iterative Monte-Carlo SURE [Vonesch et al. '08, Giryes et al. '11, Ramani et al. '12, Deledalle et al. '12]

$$\mathrm{SURE}_\theta^{(k),\mathrm{MC}}(y) = \|y - \mu_\theta^{(k)}(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta^{(k),\mathrm{MC}}(y) \qquad \widehat{\mathrm{df}}_\theta^{(k),\mathrm{MC}}(y) = \langle \mathrm{d}w_\theta^{(k)}, \, z \rangle$$

Fifty shades of SURE — continued

DoF, Monte-Carlo DoF and Iterative Monte-Carlo DoF

$$\widehat{\mathrm{df}}_\theta(y) = \mathrm{trace}(\mathrm{Jac}_{\hat\mu_\theta}(y)) \qquad \widehat{\mathrm{df}}_\theta^{\mathrm{MC}}(y) = \langle \mathrm{Jac}_{\hat\mu_\theta}(y) z,\ z\rangle \qquad \widehat{\mathrm{df}}_\theta^{(k),\mathrm{MC}}(y) = \langle \mathrm{d}w_\theta^{(k)},\ z\rangle$$

Finite-difference SURE [Ye '98, Shen-Ye '02, Ramani et al. '08]

$$\widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y) = \frac{1}{\delta}\sum_{i=1}^{n} (\hat\mu_\theta(y+\delta \mathbf{e}_i) - \hat\mu_\theta(y))_i$$

If $\hat\mu_\theta$ Lipschitz-continuous

$$\lim_{\delta\to 0} \widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y) = \widehat{\mathrm{df}}_\theta(y)$$

Issues:

- numerical instabilities
- observation dimension

Finite-difference Monte-Carlo SURE

$$\widehat{\mathrm{df}}_\theta^{\mathrm{FDMC}}(y) = \frac{1}{\delta}\langle \hat\mu_\theta(y+\delta z) - \hat\mu_\theta(y),\ z\rangle$$

$$\mathbb{E}_z\left(\widehat{\mathrm{df}}_\theta^{\mathrm{FDMC}}(y)\right) = \widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y)$$

Issue: accessibility of the true estimator!

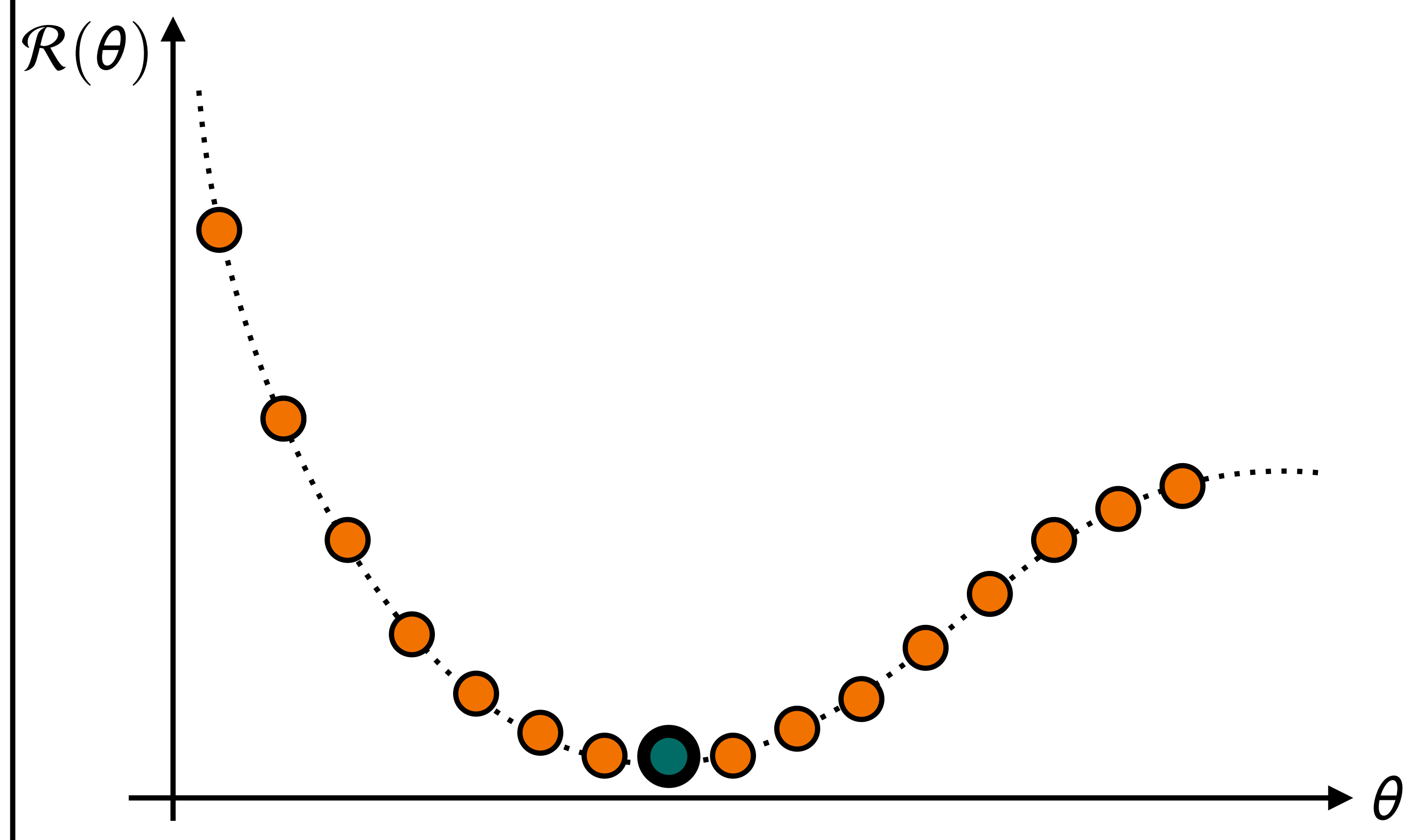
Iterative Finite-difference Monte-Carlo SURE

$$\widehat{\mathrm{df}}_\theta^{(k),\mathrm{FDMC}}(y) = \tfrac{1}{\delta}\langle \mu_\theta^{(k)}(y+\delta z) - \mu_\theta^{(k)}(y),\ z\rangle$$

Reminder: 0-order vs 1-order search

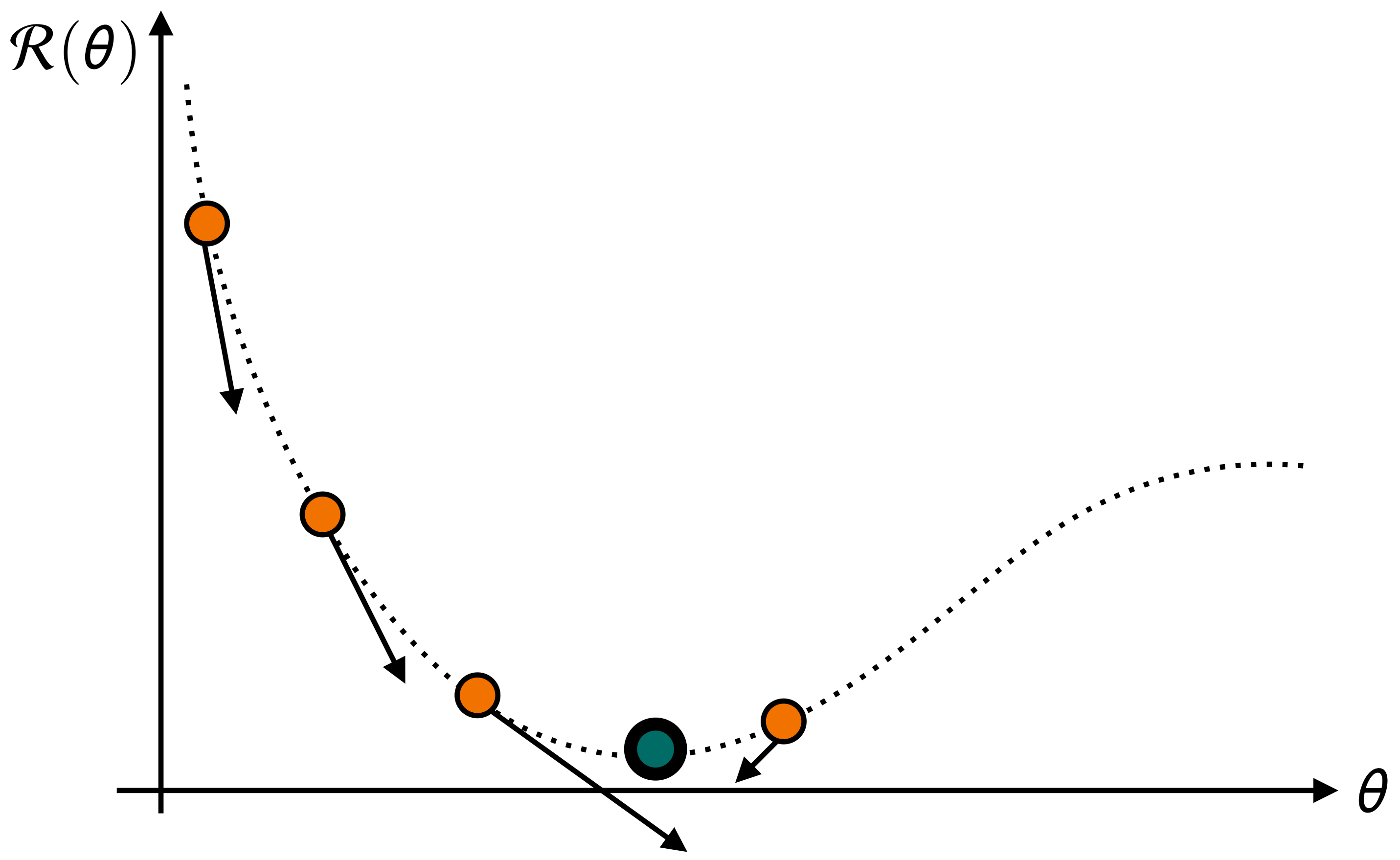
Grid search

1. Choose a criterion $\mathcal{R}$
2. Sample uniformly Θ
3. Evaluate $\mathcal{R}(\theta)$ on the grid
4. Keep the best $\theta^\star$



Hyper-gradient descent

1. Choose a criterion $\mathcal{R}$
2. Take a starting point
3. Eval. $\mathcal{R}(\theta), \nabla\mathcal{R}(\theta)$ on-the-fly
4. Keep the last iterate $\theta^\star$



BUT

$$\theta \mapsto \mathbb{E}_\varepsilon\left(\|\hat{\mu}_\theta(y) - X w_{\text{true}}\|_2^2\right)$$

(weakly) differentiable

$$\not\Downarrow$$

$$\theta \mapsto \mathrm{SURE}_\theta(y)$$

differentiable or continuous

What about $\mathrm{SURE}_\theta^{\mathrm{FD}}(y)$, $\mathrm{SURE}_\theta^{\mathrm{FDMC}}(y)$?

From SURE to SUGAR

$$\widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y) = \frac{1}{\delta}\sum_{i=1}^{n}\left(\hat{\mu}_\theta(y+\delta\mathbf{e}_i) - \hat{\mu}_\theta(y)\right)_i \qquad \widehat{\mathrm{df}}_\theta^{\mathrm{FDMC}}(y) = \frac{1}{\delta}\langle \hat{\mu}_\theta(y+\delta z) - \hat{\mu}_\theta(y),\, z\rangle$$

Proposition [Deledalle et al. '14, Pascal et al. '20]

Assume $(y,\theta) \mapsto \hat{\mu}_\theta(y)$ weakly differentiable *w.r.t* y and θ

Given $\delta > 0$, $\widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y)$, $\widehat{\mathrm{df}}_\theta^{\mathrm{FDMC}}(y)$ are also weakly differentiable

$\mathrm{SURE}_\theta^{\mathrm{FD}}(y)$, $\mathrm{SURE}_\theta^{\mathrm{FDMC}}(y)$

Stein Unbiased GrAdient estimator of the Risk (SUGAR)

$$\mathrm{SUGAR}_\theta^{\mathrm{FD/FDMC}}(y) = \nabla_\theta\left(\mathrm{SURE}_\bullet^{\mathrm{FD/FDMC}}(\bullet)\right)(y,\theta)$$

$$= 2\mathrm{Jac}_{\hat{\mu}_\bullet(\theta)}(y)^\top(\hat{\mu}_\theta(y) - y) + 2\sigma^2\nabla_\theta\left(\widehat{\mathrm{df}}_\bullet^{\mathrm{FD/FDMC}}(\bullet)\right)(y,\theta)$$

$$\nabla_\theta\left(\widehat{\mathrm{df}}_\bullet^{\mathrm{FD}}(\bullet)\right)(y,\theta) = \frac{1}{\delta}\sum_{i=1}^{n}\left(\mathrm{Jac}_{\hat{\mu}_\bullet(y+\delta\mathbf{e}_i)}(\theta) - \mathrm{Jac}_{\hat{\mu}_\bullet(y)}(\theta)\right)^\top \mathbf{e}_i$$

$$\nabla_\theta\left(\widehat{\mathrm{df}}_\bullet^{\mathrm{FDMC}}(\bullet)\right)(y,\theta) = \frac{1}{\delta}\left(\mathrm{Jac}_{\hat{\mu}_\bullet(y+\delta z)}(\theta) - \mathrm{Jac}_{\hat{\mu}_\bullet(y)}(\theta)\right)^\top z$$

Asymptotic unbiasedness of SUGAR

Theorem [Deledalle et al. '14, Pascal et al. '20]

Assume $(y, \theta) \mapsto \hat{\mu}_\theta(y)$ Lipschitz-continuous *w.r.t* y and θ

$$\lim_{\delta \to 0} \mathbb{E}_\varepsilon \left(\mathrm{SUGAR}_\theta^{\mathrm{FD/FDMC}}(y) \right) = \nabla_\theta \mathbb{E}_\varepsilon \left(\|\hat{\mu}_\bullet(y) - X w_{\mathrm{true}}\|_2^2 \right)(\theta)$$

In practice, δ / n need to not decrease quickly to ensure numerical stability

Stein Unbiased GrAdient estimator of the Risk (SUGAR)

$$\begin{aligned} \mathrm{SUGAR}_\theta^{\mathrm{FD/FDMC}}(y) &= \nabla_\theta (\mathrm{SURE}_\bullet{}^{\mathrm{FD/FDMC}}(\bullet))(y, \theta) \\ &= 2 \mathrm{Jac}_{\hat{\mu}_\bullet(\theta)}(y)^\top (\hat{\mu}_\theta(y) - y) + 2\sigma^2 \nabla_\theta (\widehat{\mathrm{df}}_\bullet{}^{\mathrm{FD/FDMC}}(\bullet))(y, \theta) \end{aligned}$$

$$\nabla_\theta (\widehat{\mathrm{df}}_\bullet{}^{\mathrm{FDMC}}(\bullet))(y, \theta) = \frac{1}{\delta} \left(\mathrm{Jac}_{\hat{\mu}_\bullet(y + \delta z)}(\theta) - \mathrm{Jac}_{\hat{\mu}_\bullet(y)}(\theta) \right)^\top z$$

SUGAR for iterative estimators

Iterative estimators $w_\theta^{(k)}(y)$

$$\mathrm{T} : \mathbb{R}^p \times \mathbb{R}^n \to \mathbb{R}^p$$

$$\begin{cases} w_\theta^{(k+1)}(y) & = \mathrm{T}(w_\theta^{(k)}(y), y) \\ \mathrm{d}w_\theta^{(k+1)}(y) & = \partial_1 \mathrm{T}(w_\theta^k(y), y) \cdot \mathrm{d}w_\theta^{(k)}(y) + \partial_2 \mathrm{T}(w_\theta^k(y), y) z \end{cases}$$

Running time x2

Global complexity: **4x** original iterative estimator

Iterative SUGAR Finite-difference + Monte-Carlo

$$\mathrm{SUGAR}_\theta^{(k),\mathrm{FD/FDMC}}(y) = \nabla_\theta(\mathrm{SURE}_\bullet{}^{(k),\mathrm{FD/FDMC}}(\bullet))(y, \theta)$$

$$= 2\mathrm{Jac}_{\mu_\bullet{}^{(k)}(\theta)}(y)^\top(\mu_\theta^{(k)}(y) - y) + 2\sigma^2 \nabla_\theta(\widehat{\mathrm{df}}_\bullet{}^{(k),\mathrm{FD/FDMC}}(\bullet))(y, \theta)$$

$$\nabla_\theta(\widehat{\mathrm{df}}_\bullet{}^{(k),\mathrm{FDMC}}(\bullet))(y, \theta) = \frac{1}{\delta}(\mathrm{d}w_\theta{}^{(k)}(y + \delta z) - \mathrm{d}w_\theta{}^{(k)}(y))$$

Running time x2

SUGAR in practice: image deblurring

Total variation deblurring

$$y = X w_{\text{true}} + \varepsilon$$

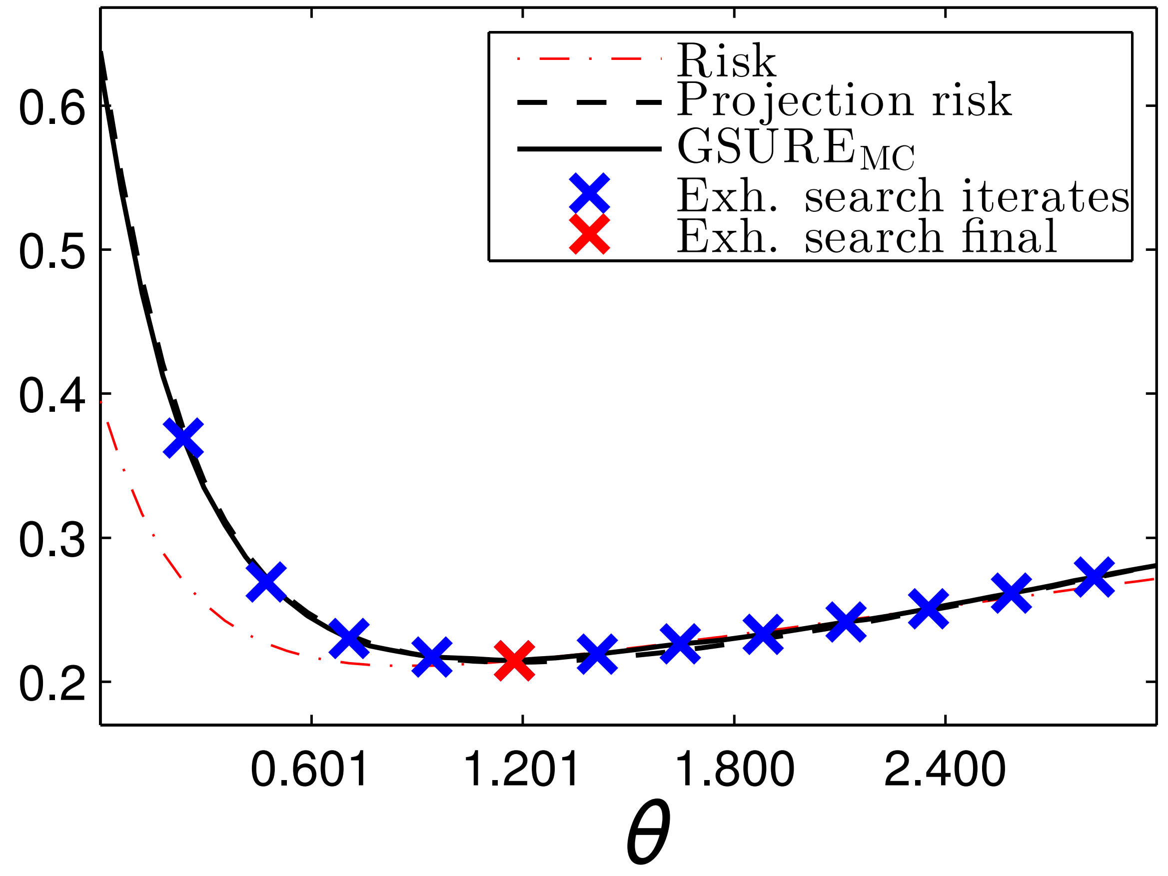
$$\hat{w}_\theta(y) \in \underset{w}{\operatorname{argmin}} \frac{1}{2}\|y - X w_{\text{true}}\|_2^2 + \theta \|\nabla_{2D} w\|_{1,2}$$

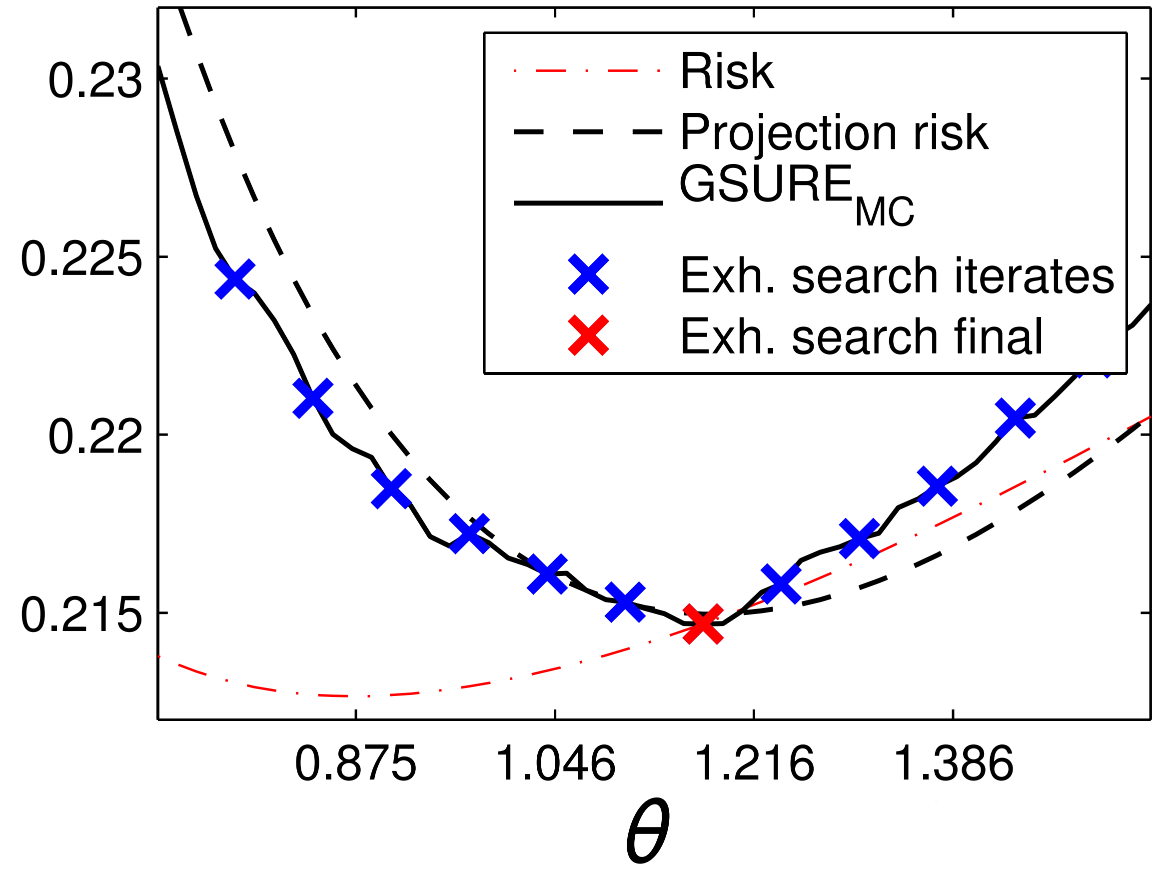
[Chambolle-Pock ’11]

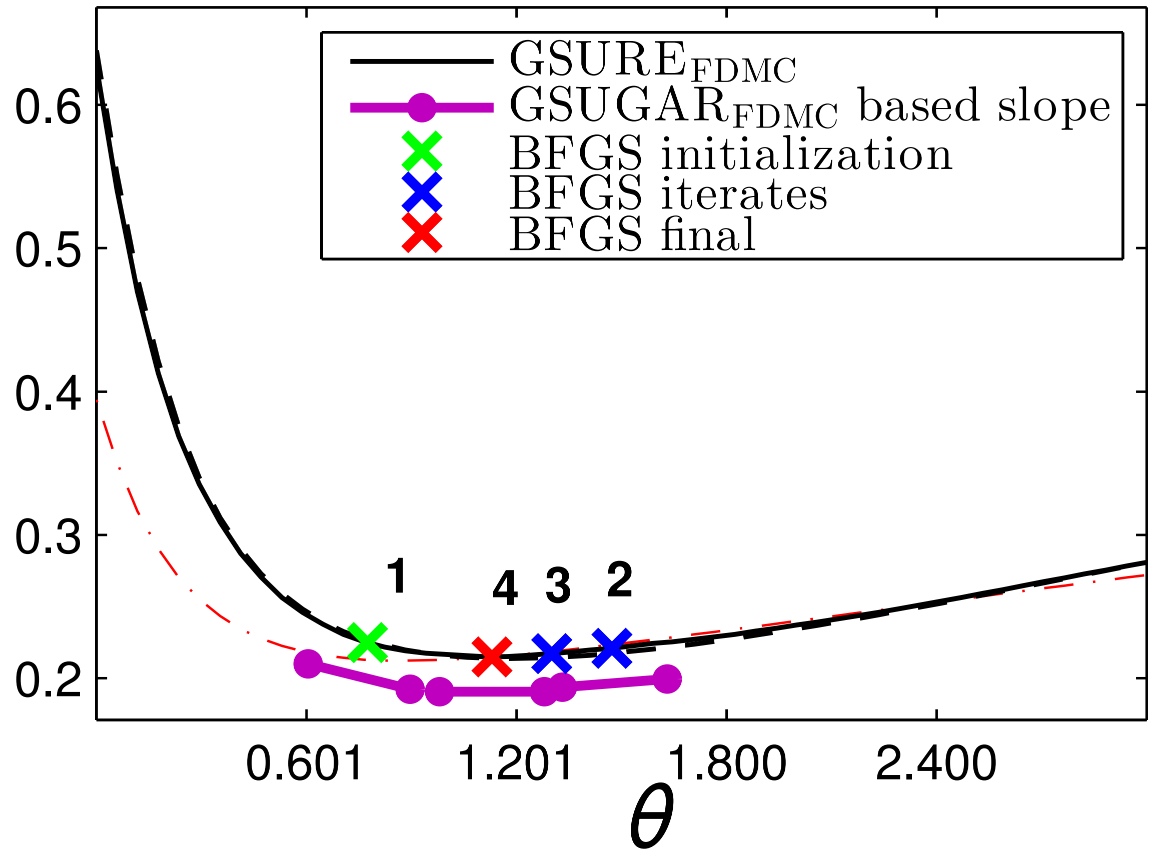
$w_\theta^{(k)}(y)$ computed with a differentiated Primal-Dual algorithm

BFGS optimization

$$\theta^{(t+1)} = \theta^{(t)} - B^{(t)} \text{SUGAR}_{\theta^{(t)}}^{(k),\text{FDMC}}(y)$$







w_{true}

y

$\hat{w}_{\theta^\star}$

Summary

Estimator

$\hat{w}_\theta : \mathbb{R}^n \longrightarrow \mathbb{R}^p$ estimator

$\theta \in \Theta$ hyper-parameter

$\mathcal{R} : \Theta \longrightarrow \mathbb{R}$ criterion

Goal

$$\text{Find } \theta^\star \in \operatorname*{argmin}_{\theta \in \Theta} \mathcal{R}(\theta)$$

(or close to it)

Estimator and algorithm

$$w_\theta^{(k)}(y) \longrightarrow \hat{w}_\theta(y)$$

$$\mathrm{Jac}_{\hat{w}_\theta}(y) \longrightarrow \mathrm{Jac}_{w_\theta^{(k)}}(y)$$

Iterative estimators

$$\mathrm{T} : \mathbb{R}^p \times \mathbb{R}^n \longrightarrow \mathbb{R}^p$$

$$\begin{cases} w_\theta^{(k)}(y) \xrightarrow{k \to +\infty} \hat{w}_\theta(y) \\ w_\theta^{(k+1)}(y) = \mathrm{T}(w_\theta^{(k)}(y), y) \end{cases}$$

Chain rule

$$\mathrm{Jac}_{w_\theta^{k+1}}(y) = \partial_1 \mathrm{T}(w_\theta^k(y), y) \cdot \mathrm{Jac}_{w_\theta^k(y)}(y) + \partial_2 \mathrm{T}(w_\theta^k(y), y)$$

"Hyper"-gradient descent

$$\theta^{k+1} = \theta^k - \rho \nabla \mathcal{R}(\theta^k)$$

Several strategies:

- Implicit differentiation
- Risk estimation (SUGAR)
- Direct Jacobian estimation