Fourier Analysis and Swarm Intelligence for Stochastic Optimization of Discrete Functions

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Overview

A new methodology for solving discrete optimization problems by the continuous approach

Discrete Fourier analysis & Particle Swarm Optimization

- Introduction
- Computational method
- Simulations
- Case studies

Introduction

- Discrete optimization: Maximization or minimization of a discrete objective function over a set of feasible parameter values where the objective function cannot be evaluated analytically
- Combinatorial methods
- Continuous methods
  - Simplicial-based cum Sample Average Approximation approach (Goyal and Ierapetritou)
  - Support vector machines to learn efficient set of multiple objective discrete optimization problem (Aytug and Sayin)

Pardalos, P.M.; Romeijin, H.E; Tuy, H. Recent developments and trends in global optimization. *Journal of Computational and Applied Mathematics* **2000**, *124*, 209-228.
Goyal, V.; Ierapetritou, M.G. Stochastic MINLP optimization using simplicial approximation. *Computers and Chemical Engineering* **2007**, *31*, 1081-1087.
Aytug, H.; Sayin, S. Using support vector machines to learn the efficient set in multiple objective discrete optimization. *European Journal of Operational Research* **2009**, *193*, 510-519.

Introduction

- A new continuous approach to the solution of discrete optimization problems
- Derive a Fourier series representation of a discrete objective function that converts the discrete optimization problem into a continuous problem
- Apply a stochastic global optimization method to solve the continuous problem

Computational Method: Discrete Fourier Analysis

- **The sampling theorem: If the Fourier transform of a function *f(x)* is zero for all frequencies greater than f_c, then the continuous function *f(x)* can be uniquely determined from its sampled values**
- **Consider a discrete function containing *N* data points for which the corresponding continuous function is to be determined.**
- **f_c: The smallest interval between any two adjacent data points**
- **Period: Domain of the discrete function**

Computational Method: Discrete Fourier Analysis

- **By the convolution theorem, values of discrete Fourier transform of the discrete function will be equal to the coefficients of the Fourier series expansion of the corresponding continuous function**
- **The following expression for the double Fourier sine series of a continuous two-dimensional function may be derived from its discrete counterpart:**

$$f(x,y)=\sum_{m=1}^{M}\sum_{n=1}^{N}a_{mn}\sin\left(\frac{m\pi x}{L_x}\right)\sin\left(\frac{n\pi y}{L_y}\right)$$

$$a_{mn}=\frac{4}{MN}\sum_{h=1}^{M}\sum_{k=1}^{N}f\left(\frac{h}{M},\frac{k}{N}\right)\sin\left(\frac{m\pi h}{M}\right)\sin\left(\frac{n\pi k}{N}\right)$$

Computational Method: Particle Swarm Optimization

- Particle Swarm Optimization (PSO) is a population-based search algorithm based on simulation of the social behavior of birds in a flock
- Particles are flown through a hyperdimensional search space
- Behavior of each particle is influenced by its own experience as well as those of its neighbors
- A kind of symbiotic cooperative algorithm
- Based on social-psychological tendency of individuals to emulate success of other individuals

Engelbrecht, A.P. Computational Intelligence An Introduction. England: John Wiley & Sons Ltd, 2002.
Kennedy, J.; Eberhart, R.C. Particle Swarm Optimization. *Proceedings of the IEEE International Conference on Neural Networks* **1995**, *4*, 1942.

Computational Method: Particle Swarm Optimization

- **Position of each particle, P_i, in the swarm is updated at each time step:**

$$x_i(t) = x_i(t-1) + v_i(t)$$

where x: position, v: velocity

- **Velocity of each particle is updated at each time step:**

$$v_i(t) = \varphi v_i(t-1) + \rho_1\{x_{pbest,i} - x_i(t-1)\} + \rho_2\{x_{gbest} - x_i(t-1)\}$$

where φ: inertia weight, ρ: random variable

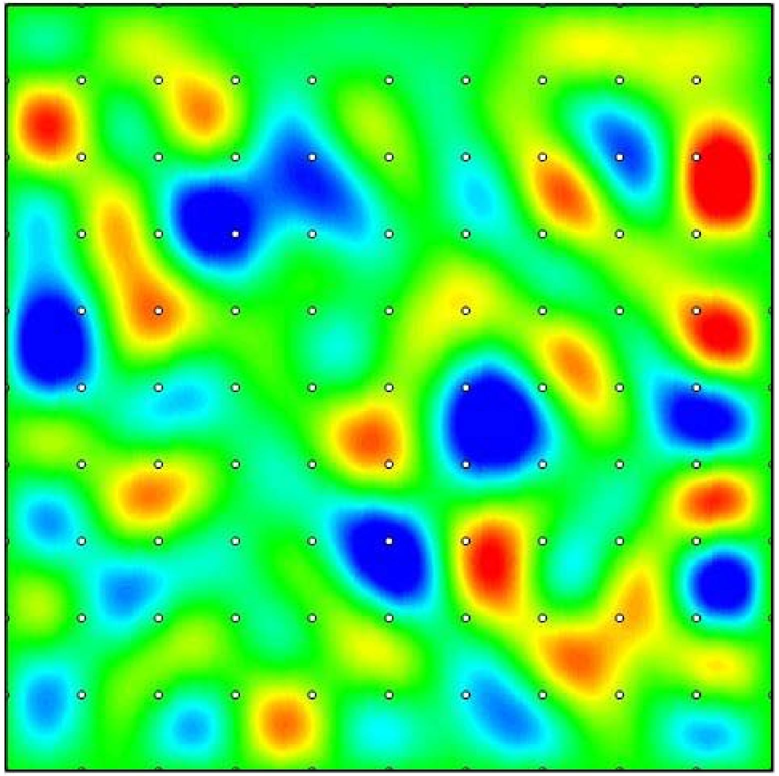
- **To ensure convergence, the following must hold:**

$$\varphi > \frac{1}{2}(c_1 + c_2) - 1$$

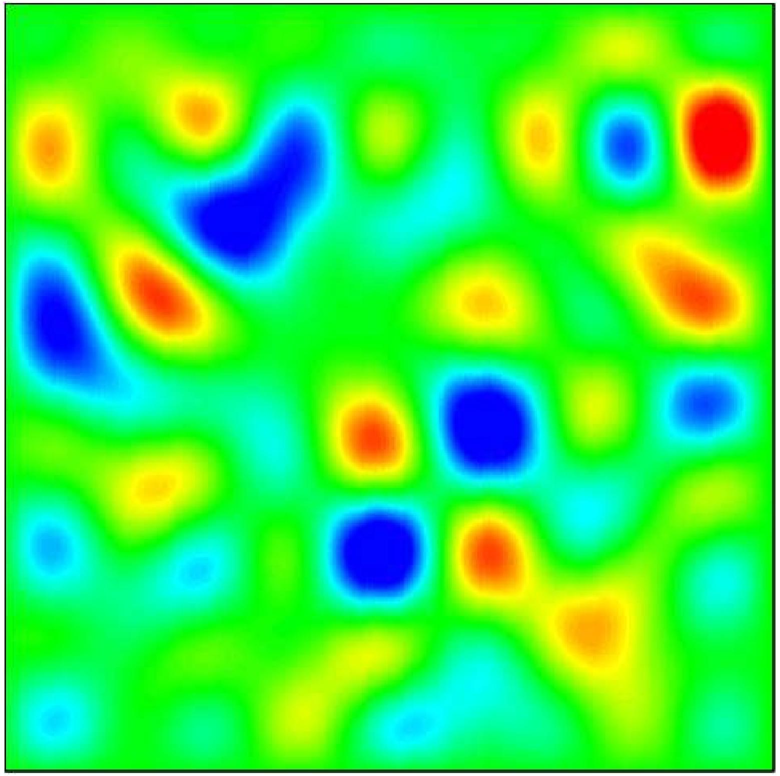
Simulations

- **Number of data points = 100**

Original



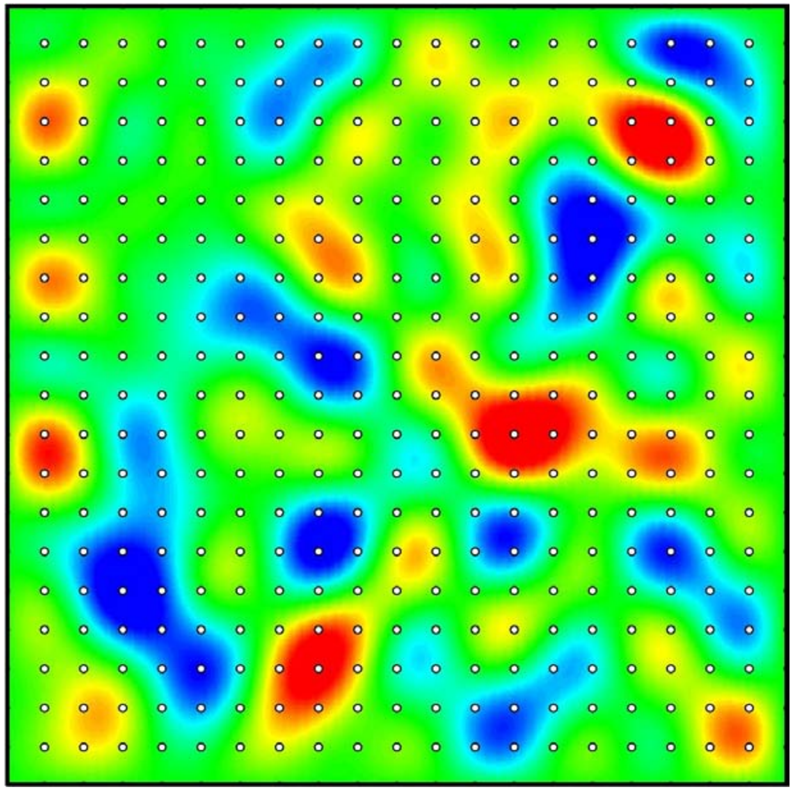
Reconstructed



Simulations

- **Number of data points = 400**

Original



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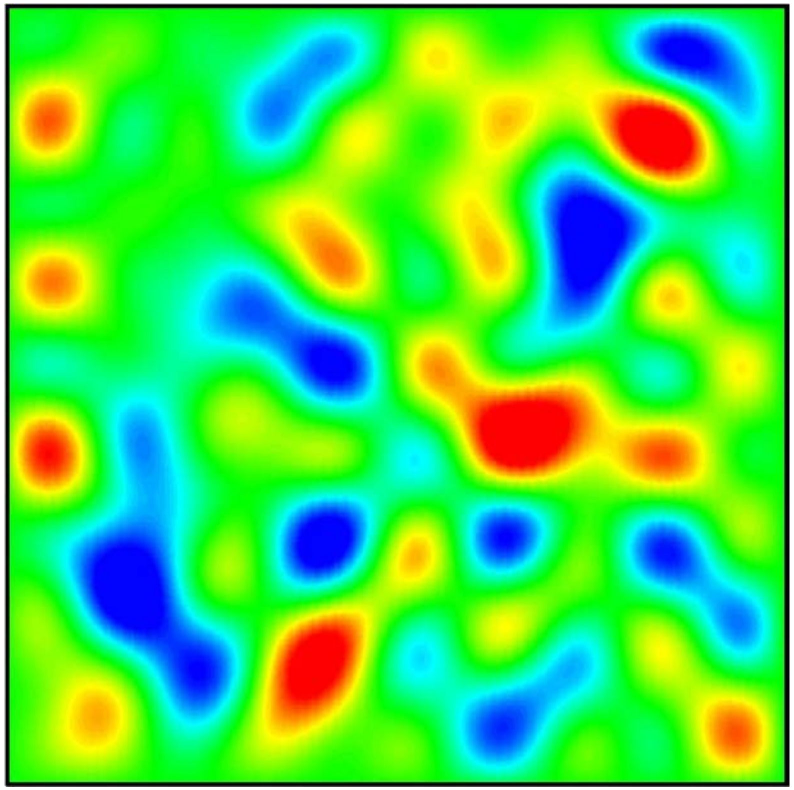

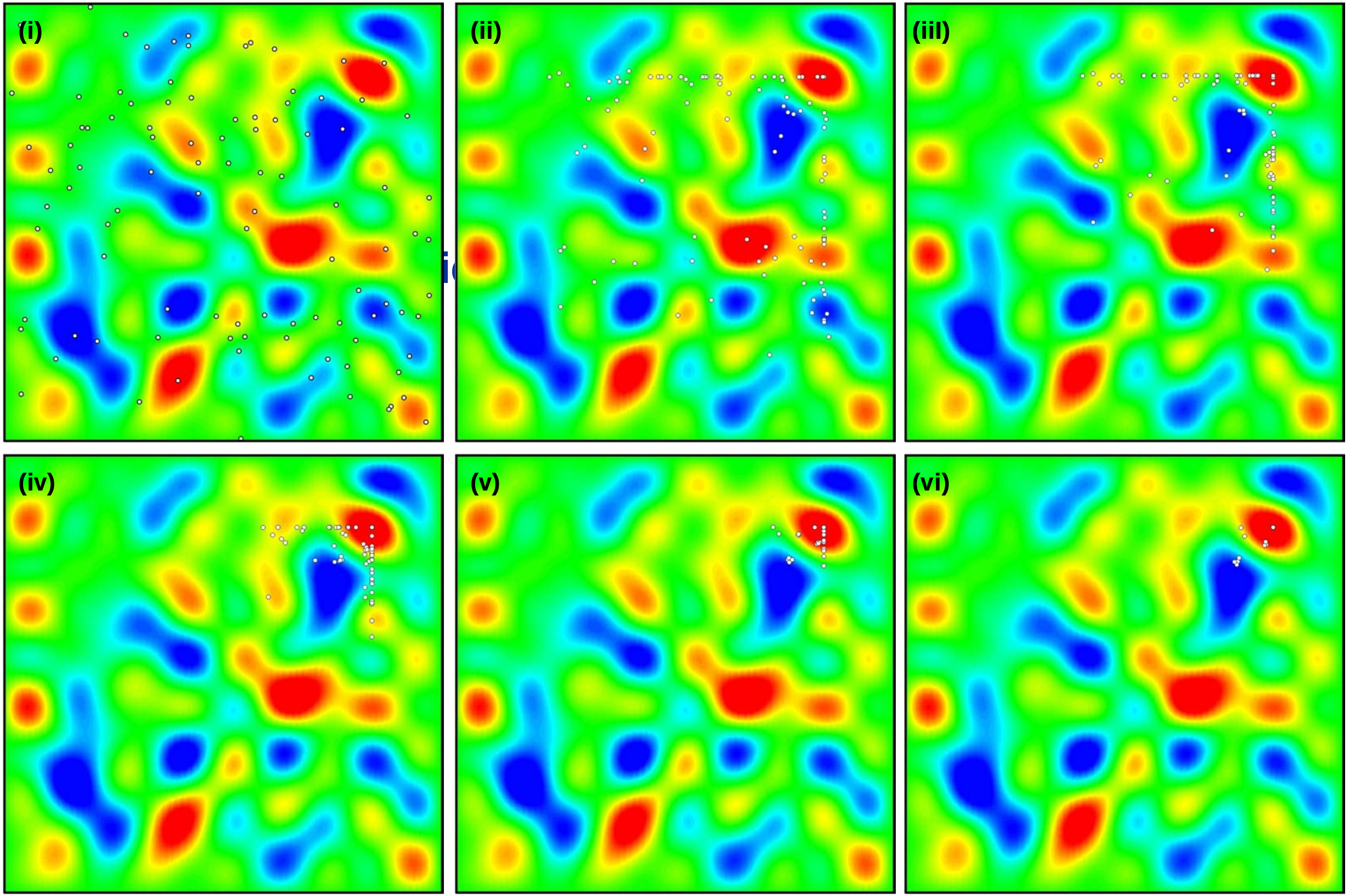
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Case studies

- **Based on experimental work conducted by Giannakou *et al.*, Lee and Gilmore and Tabandeh *et al.***
- **Each used response surface methodology and a full factorial design for the experiments**
- **Tabandeh *et al.* investigated dry cell weight at the time of induction and inducer concentration required to maximize the productivity of a human interferon beta by the recombinant bacteria *Escherichia coli* in high cell density culture**

Giannakou, S.A.; Dallas, P.P.; Rekkas, D.M.; Choulis, N.H. In vitro evaluation of nimodipine permeation through human epidermis using response surface methodology. *International Journal of Pharmaceutics* **2002**, *241*, 27–34.
Lee, K.; Gilmore, D.F. Statistical experimental design for bioprocess modeling and optimization analysis: Repeated-measures method for dynamic biotechnology process. *Applied Biochemistry and Biotechnology* **2006**, *135*, 101-115.
Tabandeh, F.; Khodabandeh, M.; Yakhchali, B.; Habib-Ghomi, H.; Shariati, P. Response surface methodology for optimizing the induction conditions of recombinant interferon beta during high cell density culture. *Chemical Engineering Science*, **2008,** *63,* 2477-2483.

Case studies

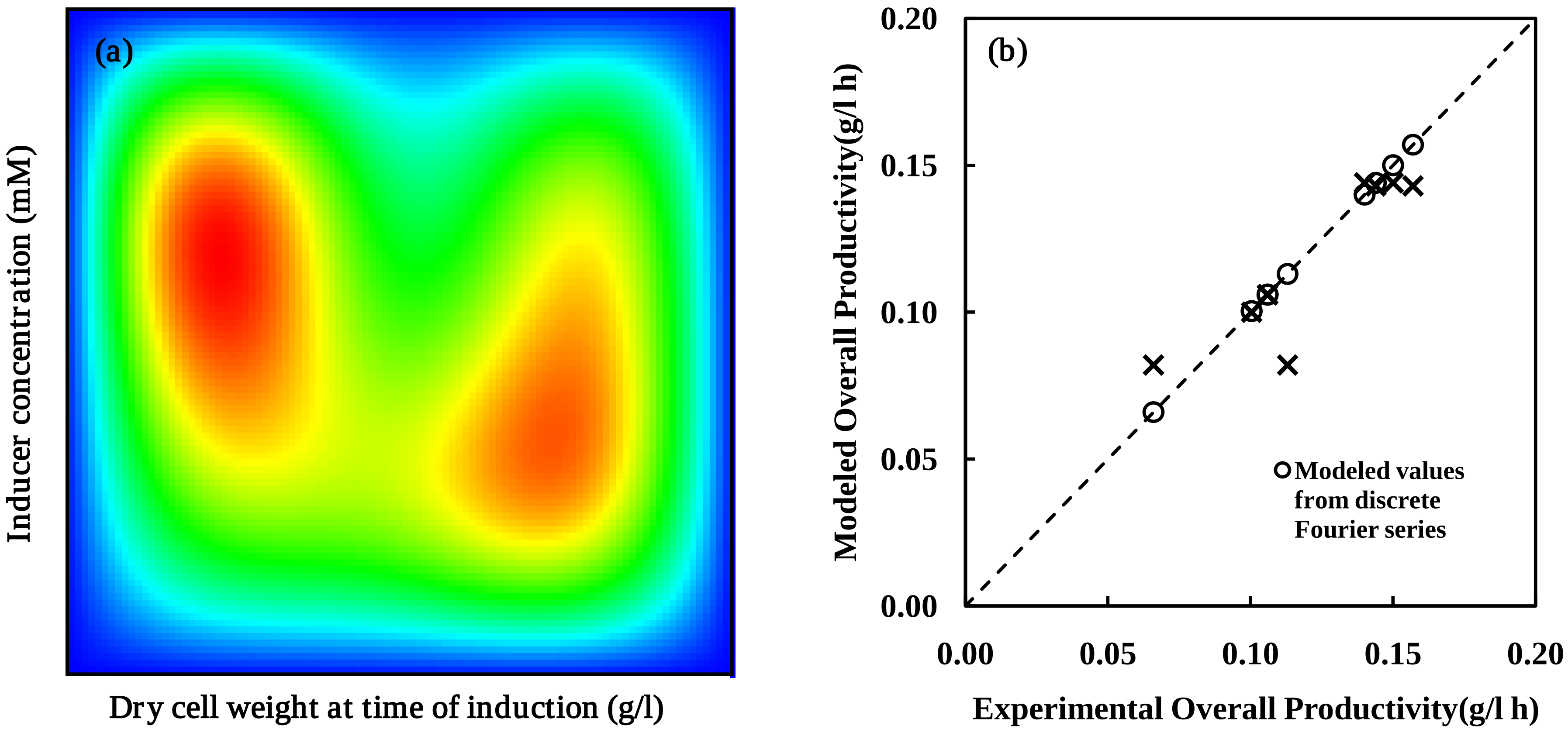
Variables	Symbol	Coded levels		
		−1 (low)	0 (mid)	+1 (high)
DCW at the time of induction (g/l)	*A*	50	60	70
Inducer (IPTG) concentration (mM)	*B*	1	2	3

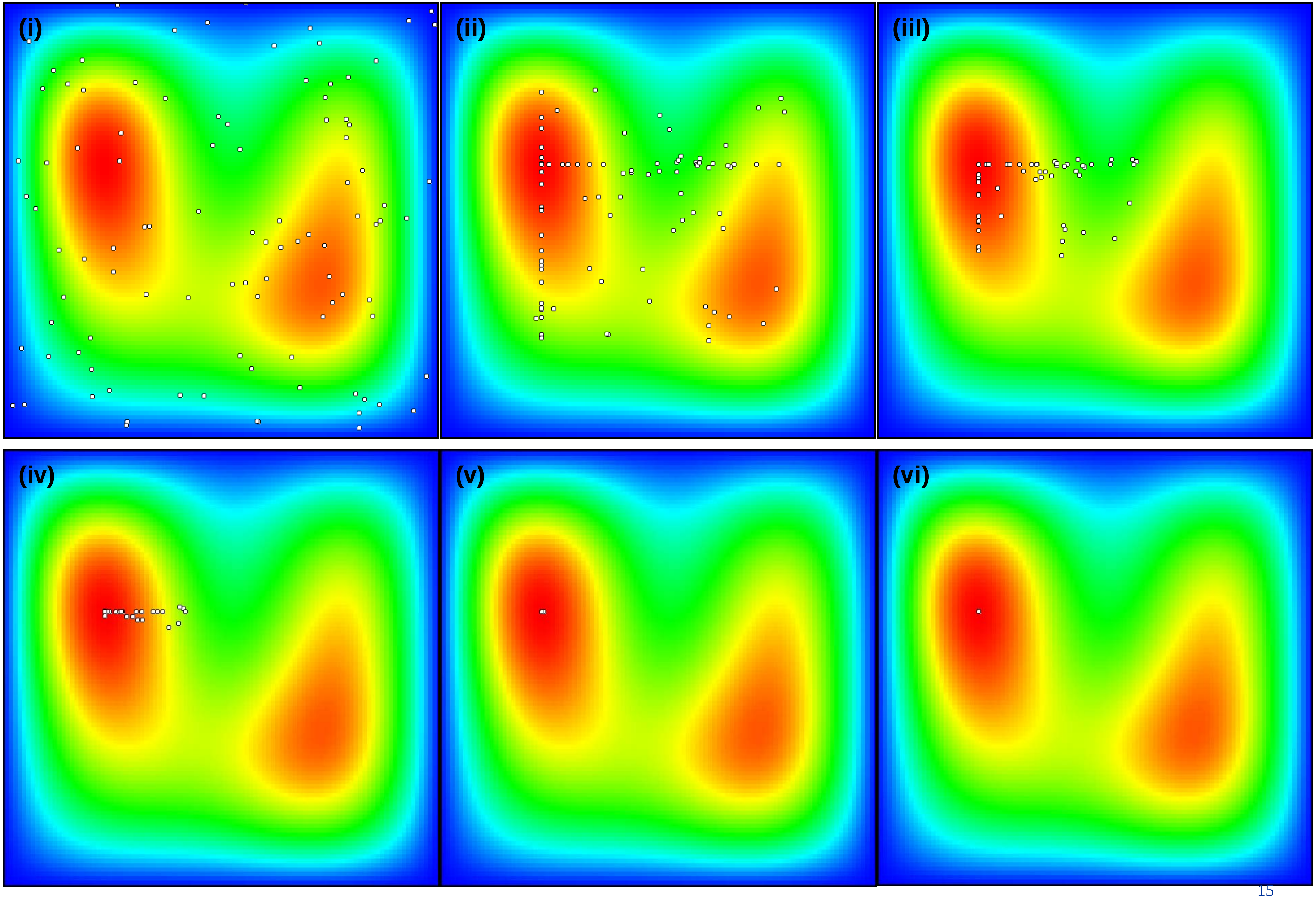
Trial no.	*A*	*B*	Overall productivity (g/l h)
1	−1	−1	0.106
2	0	−1	0.113
3	+1	−1	0.140
4	−1	0	0.157
5	0	0	0.093
6	+1	0	0.144
7	−1	+1	0.150
8	0	+1	0.066
9	+1	+1	0.106
10	0	0	0.090
11	0	0	0.113
12	0	0	0.100
13	0	0	0.106

Tabandeh, F.; Khodabandeh, M.; Yakhchali, B.; Habib-Ghomi, H.; Shariati, P. Response surface methodology for optimizing the induction conditions of recombinant interferon beta during high cell density culture. *Chemical Engineering Science*, **2008,** *63,* 2477-2483.

Case studies

- **Comparison of values of modeled overall productivity from original study and from current study**

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Case studies

Variable	Tabandeh *et al.* 1	Tabandeh *et al.* 2	Current study
Dry cell weight (g/l)	50	70	49.3
Inducer concentration (mM)	2.54	1.29	2.51
Overall productivity (g/l h)	0.151	0.151	0.167

Case studies

- Locate global optimal solutions that may not correspond to any of the original experimental data points
- Corroborate the optimal solutions obtained with response surface methodology
- Provide supplementary set of optimal solutions that response surface methodology may have missed

Conclusions

- Successful application of discrete Fourier series method coupled with PSO algorithm to:
  - Simulated discrete objective functions
  - Experimental data of productivity of recombinant human interferon beta
- Possible to alter current methodology for other experimental designs like central composite design
- Possible to extend current methodology to higher dimensions

Acknowledgement

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Thank you

- **Q&A**

Thank you

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Case studies

- **Lee & Gilmore investigated concentration level of carbon source and fermentation time required for optimal lipid production**

Lee, K.; Gilmore, D.F. Statistical experimental design for bioprocess modeling and optimization analysis: Repeated-measures method for dynamic biotechnology process. *Applied Biochemistry and Biotechnology* **2006**, *135*, 101-115.

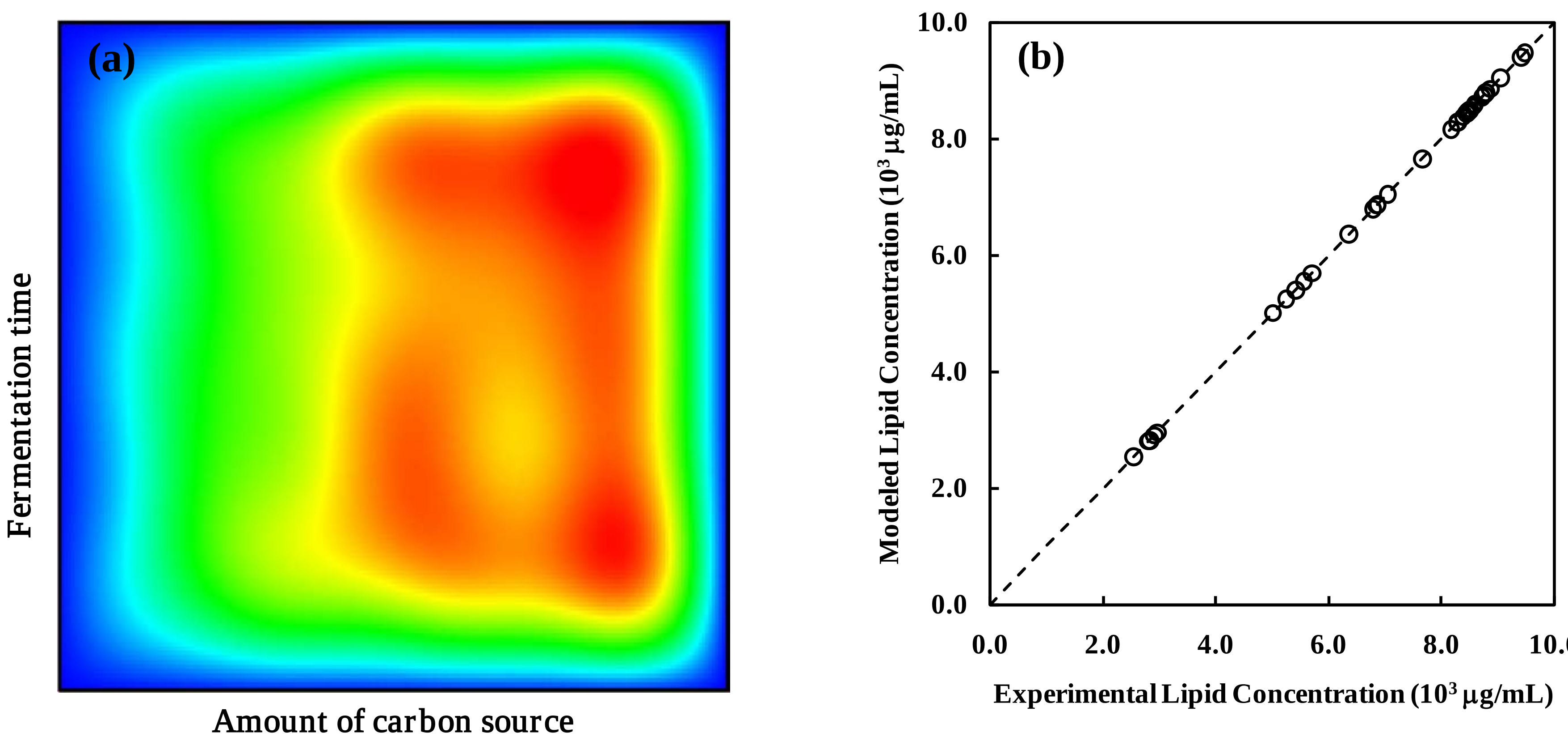
Case studies

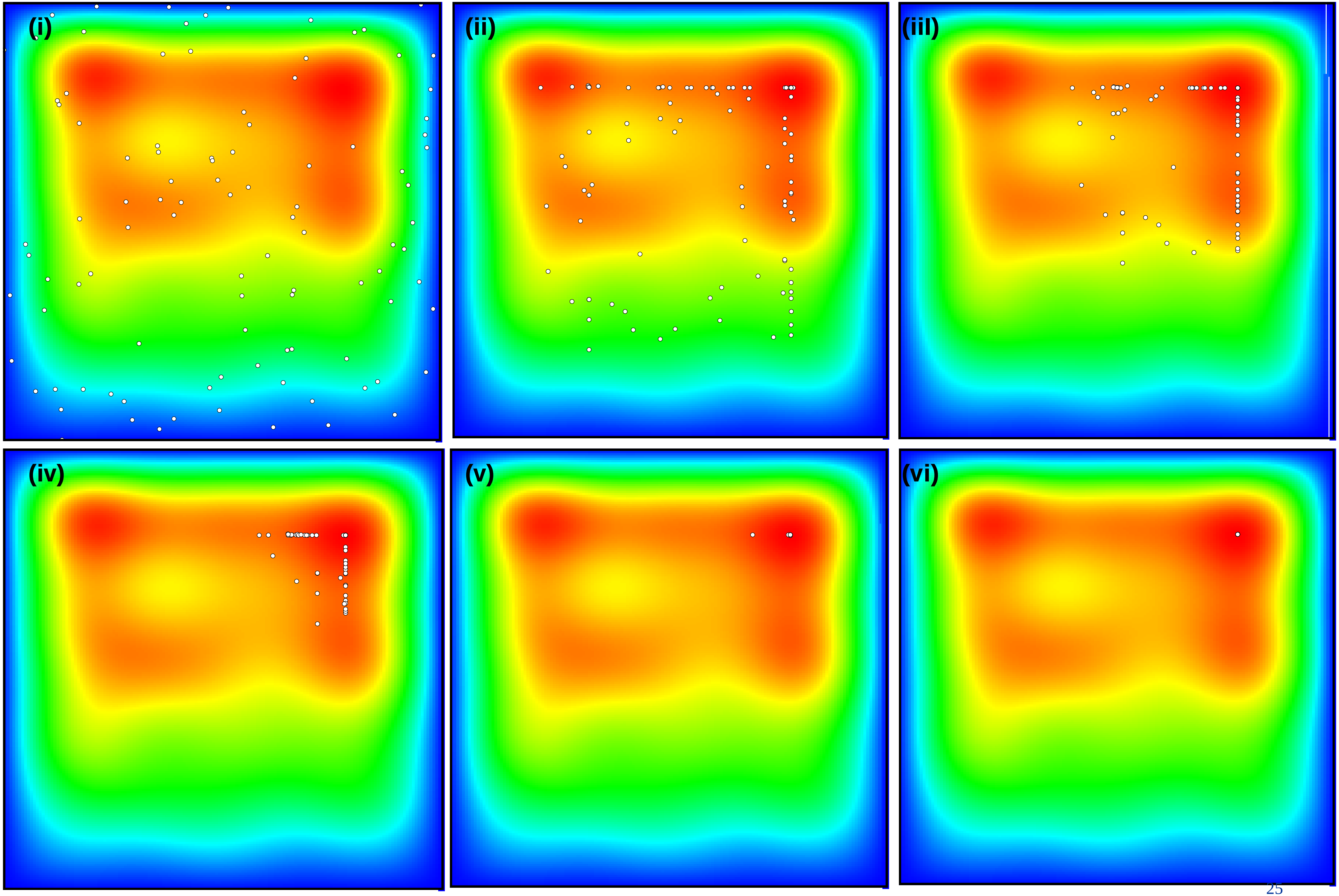
Table 1
Layout of Repeated-Measures and Results

Response: lipid (µg/mL)								
Treatment: C[a]-source (mL)	Subject: bioreactor	Repeated factor: time (h)						
		24	48	72	96	120	144	168
30	# 1	2910	5560	6870	7660	8280	8590	8860
30	# 2	3120	5260	7260	8040	8340	9150	9220
35	# 1	2830	5700	7050	9050	8440	8500	8560
35	# 2	2860	5380	7140	9050	8500	8610	8720
40	# 1	2960	5410	6860	8510	8380	8720	8290
40	# 2	3130	5510	7220	8500	8590	8700	8630
45	# 1	2540	5250	6790	8170	8760	9410	8460
45	# 2	2520	5180	6890	8630	9030	9280	8910
50	# 1	2810	5010	6360	8470	8790	9480	8460
50	# 2	2670	5130	6570	8910	9040	9680	8930

Lee, K.; Gilmore, D.F. Statistical experimental design for bioprocess modeling and optimization analysis: Repeated-measures method for dynamic biotechnology process. *Applied Biochemistry and Biotechnology* **2006**, *135*, 101-115.

Case studies

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Case studies

Variable	Lee & Gilmore	Current study
Carbon source (mL)	50.00	48.32
Fermentation time (h)	140	154
Lipid production (µg/mL)	9200	10489